Quantum Mechanics

Mathematical Structure and Physical Structure

Part 2

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Chapter 11

Time-Dependent Perturbation Theory

11.1 Theory

Time-independent or stationary-state perturbation theory, as we developed earlier, allows us to find approximations for the energy eigenvalues and eigenvectors in complex physical systems that are not solvable in closed form and where we could write \hat{H} in two parts as

$$\hat{H} = \hat{H}_0 + \hat{V}$$
 (11.1)

For these perturbation methods to work, \hat{V} must be *weak* and *time-independent*.

We now turn our attention to the case

$$\hat{H} = \hat{H}_0 + \hat{V}_t \tag{11.2}$$

where \hat{V}_t is weak and time-dependent.

Examples might be the decays of an atomic system by photon emission or the ionization of an atom by shining light on it.

We assume that at some time t_0 the system has evolved into the state $|\psi_t^{(0)}\rangle$, i.e., the state $|\psi_t^{(0)}\rangle$ satisfies the time evolution equation

$$i\hbar\frac{\partial}{\partial t}\left|\psi_{t}^{(0)}\right\rangle = \hat{H}_{0}\left|\psi_{t}^{(0)}\right\rangle \qquad t \le t_{0} \tag{11.3}$$

It is a solution of the time-dependent Schrödinger equation with no perturbing interactions before t_0 where

$$\hat{H} = \hat{H}_0 \qquad t \le t_0 \tag{11.4}$$

At time t_0 we turn on the interaction potential (or perturbation) so that

$$\hat{H} = \hat{H}_0 + \hat{V}_t \qquad t \ge t_0$$
 (11.5)

The new state of the system then satisfies

$$i\hbar\frac{\partial}{\partial t}|\psi_t\rangle = \hat{H}|\psi_t\rangle = (\hat{H}_0 + \hat{V}_t)|\psi_t\rangle \qquad t \ge t_0$$
(11.6)

with the boundary condition(initial value)

$$|\psi_t\rangle = \left|\psi_t^{(0)}\right\rangle \text{ at } t = t_0 \tag{11.7}$$

As we said, we assume that the full time-dependent Schrödinger equation cannot be solved in closed form and so we look for approximate solutions.

We let \hat{V}_t be a small perturbation, i.e., we assume there is a natural small parameter in \hat{V}_t (as we saw in time-independent perturbation theory) and we make an expansion of the solution in powers of \hat{V}_t or this small parameter.

Since the effect of \hat{H}_0 will be much greater than the effect of \hat{V}_t , most of the time dependence comes from \hat{H}_0 . If we could neglect \hat{V}_t , then since \hat{H}_0 is independent of time, we would have the simple time dependence

$$\left|\psi_{t}\right\rangle = e^{-\frac{i}{\hbar}\hat{H}_{0}t}\left|\psi_{t}^{(0)}\right\rangle \tag{11.8}$$

Let us assume that this is still approximately true and remove this known time dependence from the solution. This should remove the major portion of the total time dependence from the problem. We do this by assuming a solution of the form

$$|\psi_t\rangle = e^{-\frac{i}{\hbar}H_0 t} |\psi(t)\rangle \tag{11.9}$$

and then determining and solving the equation for the new state vector $|\psi(t)\rangle$.

Substituting this assumption in our original equation, the equation for $|\psi(t)\rangle$ is then given by

$$i\hbar\frac{\partial}{\partial t}\left(e^{-\frac{i}{\hbar}\hat{H}_{0}t}|\psi(t)\rangle\right) = (\hat{H}_{0} + \hat{V}_{t})\left(e^{-\frac{i}{\hbar}\hat{H}_{0}t}|\psi(t)\rangle\right)$$
$$\hat{H}_{0}e^{-\frac{i}{\hbar}\hat{H}_{0}t}|\psi(t)\rangle + i\hbar e^{-\frac{i}{\hbar}\hat{H}_{0}t}\frac{\partial}{\partial t}|\psi(t)\rangle$$
$$= \hat{H}_{0}e^{-\frac{i}{\hbar}\hat{H}_{0}t}|\psi(t)\rangle + \hat{V}_{t}e^{-\frac{i}{\hbar}\hat{H}_{0}t}|\psi(t)\rangle$$
$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{V}(t)|\psi(t)\rangle$$
(11.10)

where

$$\hat{V}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t} \hat{V}_t e^{-\frac{i}{\hbar}\hat{H}_0 t}$$
(11.11)

The substitution has removed \hat{H}_0 from the equation and changed the time dependence of the perturbing potential. We are in the so-called *interaction picture* or representation where both the state vectors and the operators depend on time as we discussed earlier in Chapter 6.

We develop a $formal\ solution$ by integrating this equation of motion for the state vector to get

$$i\hbar \int_{t_0}^t \frac{\partial}{\partial t'} |\psi(t')\rangle dt' = \int_{t_0}^t \hat{V}(t') |\psi(t')\rangle dt'$$
$$= i\hbar (|\psi(t)\rangle - |\psi(t_0)\rangle)$$
(11.12)

so that the formal solution is given by

$$|\psi(t)\rangle = |\psi(t_0)\rangle + \frac{1}{i\hbar} \int_{t_0}^t \hat{V}(t') |\psi(t')\rangle dt'$$
(11.13)

This is an *integral equation* for $|\psi(t)\rangle$. We solve it as a power series in \hat{V}_t by the *method of iteration*.

The $0^{th}-\!\mathrm{order}$ approximation is found by neglecting the perturbing potential. We get

$$|\psi(t)\rangle = |\psi(t_0)\rangle \tag{11.14}$$

The 1^{st} -order approximation is obtained by inserting the 0^{th} -order approximation into the full equation. We get

$$|\psi(t)\rangle = |\psi(t_{0})\rangle + \frac{1}{i\hbar} \int_{t_{0}}^{t} \hat{V}(t') |\psi(t_{0})\rangle dt'$$
$$= \left(1 + \frac{1}{i\hbar} \int_{t_{0}}^{t} \hat{V}(t') dt'\right) |\psi(t_{0})\rangle$$
(11.15)

The 2^{nd} -order approximation is obtained by inserting the 1^{st} -order approximation into the full equation. We get

$$\begin{aligned} |\psi(t)\rangle &= |\psi(t_0)\rangle + \frac{1}{i\hbar} \int_{t_0}^t \hat{V}(t') |\psi(t_0)\rangle dt' \\ &+ \frac{1}{(i\hbar)^2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{V}(t') \hat{V}(t'') |\psi(t_0)\rangle \end{aligned}$$
(11.16)

Notice that in all subsequent iterations the operators $\hat{V}(t'), \hat{V}(t''), \ldots$, etc, always occur in order of increasing time from right to left.

We can write the general result as

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle \tag{11.17}$$

where

$$\hat{U}(t,t_0) = \hat{I} + \sum_{n=1}^{\infty} \frac{1}{(i\hbar)^n} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \hat{V}(t_1) \hat{V}(t_2) \dots \hat{V}(t_n)$$
(11.18)

The complete, formal solution to the problem is then given by

$$|\psi_t\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t} |\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t} \hat{U}(t, t_0) |\psi(t_0)\rangle$$
(11.19)

so that

$$e^{-\frac{i}{\hbar}\hat{H}_0t}\hat{U}(t,t_0)$$
 = the total time development operator (11.20)

Before developing the detailed techniques of time-dependent perturbation theory, let us spend some time with the operator $\hat{U}(t, t_0)$ and discuss some of its properties.

We first introduce the idea of a $time\-ordered\ product$ of operators as follows. The symbol

$$\left(\hat{A}(t)\hat{B}(t_1)\hat{C}(t_2)....\hat{X}(t_n)\right)_{+} \equiv T\left(\hat{A}(t)\hat{B}(t_1)\hat{C}(t_2)....\hat{X}(t_n)\right)$$
(11.21)

means the product of the operators where the operators are written from right to left in order of increasing times, i.e.,

$$\left(\hat{A}(t)\hat{B}(t')\right)_{+} = \begin{cases} \hat{A}(t)\hat{B}(t') & t \ge t' \\ \hat{B}(t')\hat{A}(t) & t' \ge t \end{cases}$$
(11.22)

Now, we have using the time-ordered product definition

$$\left(\left[\int_{t_0}^t \hat{V}(t') dt' \right]^2 \right)_+ = \left(\int_{t_0}^t \hat{V}(t') dt' \int_{t_0}^t \hat{V}(t'') dt'' \right)_+ \\
= \int_{t_0}^t dt' \int_{t_0}^t dt'' (\hat{V}(t') \hat{V}(t''))_+ \\
= \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{V}(t') \hat{V}(t'') + \int_{t_0}^t dt'' \int_{t_0}^{t''} dt' \hat{V}(t'') \hat{V}(t') \\
= 2 \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{V}(t') \hat{V}(t'') \qquad (11.23)$$

and in general

$$\left(\left[\int_{t_0}^t \hat{V}(t') dt' \right]^n \right)_+ = \left(\int_{t_0}^t \hat{V}(t_1) dt_1 \int_{t_0}^t \hat{V}(t_2) dt_2 \dots \int_{t_0}^t \hat{V}(t_n) dt_n \right)_+$$
$$= \int_{t_0}^t dt_1 \int_{t_0}^t dt_2 \dots \int_{t_0}^t dt_n (\hat{V}(t_1) \hat{V}(t_2) \dots \hat{V}(t_n))_+$$
$$= n! \int_{t_0}^t dt_1 \int_{t_0}^t dt_2 \dots \int_{t_0}^t dt_n \hat{V}(t_1) \hat{V}(t_2) \dots \hat{V}(t_n) \quad (11.24)$$

because there are n! possible orderings of the n terms involved. This last form is identical to the expression for $\hat{U}(t, t_0)$ and thus we have

$$\hat{U}(t,t_0) = \sum_{n=0}^{\infty} \frac{1}{(i\hbar)^n} \frac{1}{n!} \left(\left[\int_{t_0}^t \hat{V}(t') dt' \right]^n \right)_+ \\ = \left(\exp\left[-\frac{i}{\hbar} \int_{t_0}^t \hat{V}(t') dt' \right] \right)_+$$
(11.25)

The last expression is just a *convenient shorthand for the infinite sum*. In order to verify that this is in fact a solution of

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{V}(t)|\psi(t)\rangle$$
 (11.26)

we must prove that

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)|\psi(t_0)\rangle = \hat{V}(t)\hat{U}(t,t_0)|\psi(t_0)\rangle$$
(11.27)

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{V}(t)\hat{U}(t,t_0)$$
(11.28)

Substituting, we have

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_{0}) = i\hbar\frac{\partial}{\partial t}\left(\exp\left[-\frac{i}{\hbar}\int_{t_{0}}^{t}\hat{V}(t')dt'\right]\right)_{+}$$
$$=\left(\hat{V}(t)\exp\left[-\frac{i}{\hbar}\int_{t_{0}}^{t}\hat{V}(t')dt'\right]\right)_{+}$$
(11.29)

In the differentiation we do not have to worry about the non-commutation of the operators inside the time-ordered product since the *order is already specified*. Since t is certainly the latest time in the time-ordered product and therefore

all the other operators will be on the right of $\hat{V}(t)$ we can pull it outside the time-ordered product and write

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{V}(t)\left(\exp\left[-\frac{i}{\hbar}\int_{t_0}^t \hat{V}(t')dt'\right]\right)_+ = \hat{V}(t)\hat{U}(t,t_0)$$

as required.

The most important question (really the only question) that is usually asked in quantum mechanics is the following:

Suppose that the system is initially in an eigenstate $|n\rangle$ of \hat{H}_0 , i.e., $\hat{H}_0 |n\rangle = \epsilon_n |n\rangle$. What is the probability that the system will be observed, after the perturbation has had time to act, in a different (and thus orthogonal) eigenstate of \hat{H}_0 , say $|m\rangle$?

Alternatively, the question is sometimes posed this way:

What is the probability that the interaction causes the system to make a *transition* from the state $|n\rangle$ to the state $|m\rangle$?

The probability amplitude for observing the system in the state $|m\rangle$ at time t is given by

$$\langle m \mid \psi_t \rangle = \langle m \mid e^{-\frac{i}{\hbar} H_0 t} \hat{U}(t, t_0) \mid \psi(t_0) \rangle$$

= $\langle m \mid e^{-\frac{i}{\hbar} \hat{H}_0 t} \hat{U}(t, t_0) \mid n \rangle$ (11.30)

where

$$|\psi(t_0)\rangle = |n\rangle \tag{11.31}$$

is the initial state.

Setting $t_0 = 0$ for simplicity and using the 1^{st} -order approximation for $\hat{U}(t,0)$ and also using

$$\left\langle m\right|e^{-\frac{i}{\hbar}\hat{H}_{0}t} = \left(e^{\frac{i}{\hbar}\hat{H}_{0}t}\left|m\right\rangle\right)^{+} = \left(e^{\frac{i}{\hbar}\varepsilon_{m}t}\left|m\right\rangle\right)^{+} = \left\langle m\right|e^{-\frac{i}{\hbar}\varepsilon_{m}t}$$
(11.32)

we get

$$\langle m \mid \psi_t \rangle = \frac{1}{i\hbar} e^{-\frac{i}{\hbar}\varepsilon_m t} \int_0^t dt' \langle m \mid \hat{V}(t') \mid n \rangle$$

$$= \frac{1}{i\hbar} e^{-\frac{i}{\hbar}\varepsilon_m t} \int_0^t dt' \langle m \mid e^{\frac{i}{\hbar}\hat{H}_0 t} \hat{V}_{t'} e^{-\frac{i}{\hbar}\hat{H}_0 t} \mid n \rangle$$

$$= \frac{1}{i\hbar} e^{-\frac{i}{\hbar}\varepsilon_m t} \int_0^t dt' e^{\frac{i}{\hbar}(\varepsilon_m - \varepsilon_n)t} \langle m \mid \hat{V}_{t'} \mid n \rangle$$

$$(11.33)$$

The probability of the transition is then

$$P_{n \to m}(t) = \left| \langle m \mid \psi_t \rangle \right|^2 = \frac{1}{\hbar^2} \left| \int_0^t dt' e^{\frac{i}{\hbar} (\varepsilon_m - \varepsilon_n) t} \langle m \mid \hat{V}_{t'} \mid n \rangle \right|^2$$
(11.34)

The simplest example is when \hat{V}_t is not a function of t, or $\hat{V}_t = \hat{V}$. We then have

$$P_{n \to m}(t) = \left| \langle m \mid \psi_t \rangle \right|^2 = \frac{\left| \langle m \mid \hat{V}_{t'} \mid n \rangle \right|^2}{\hbar^2} \left| \int_0^t dt' e^{\frac{i}{\hbar} (\varepsilon_m - \varepsilon_n) t} \right|^2$$
(11.35)

If we define $\Delta = \epsilon_m - \epsilon_n$, then we have

$$P_{n \to m}(t) = \left| \langle m | \hat{V}_{t'} | n \rangle \right|^2 \left| \frac{1 - e^{-\frac{i}{\hbar}} \Delta t}{\Delta} \right|^2 = \left| \langle m | \hat{V}_{t'} | n \rangle \right|^2 \left(\frac{\sin \frac{\Delta t}{2\hbar}}{\Delta/2} \right)^2$$
(11.36)

for the transition probability.

11.1.1 What is the physical meaning of this result?

We must be *very careful* when we use the words

the perturbation causes a transition between eigenstates of \hat{H}_0

What this means physically is that the system has absorbed from the perturbing field (or emitted to it) the energy difference $\Delta = \epsilon_m - \epsilon_n$ and therefore the system has changed its energy.

Does the statement also mean that the state vector has changed from an initial value $|\psi(0)\rangle = |n\rangle$ to a final value $|\psi(t)\rangle = |m\rangle$?

We can get a better feeling for the correct answer to this question by deriving the result in a different manner. We have

$$i\hbar\frac{\partial}{\partial t}|\psi_t\rangle = \hat{H}|\psi_t\rangle = (\hat{H}_0 + \hat{V}_t)|\psi_t\rangle \qquad (11.37)$$

and

$$\hat{H}_0 |n\rangle = \varepsilon_n |n\rangle \tag{11.38}$$

As in our development of time-independent perturbation theory, we let

$$\hat{V}_t = g\hat{U}_t \tag{11.39}$$

where g is a small parameter.

The set of eigenvectors $\{|n\rangle\}$ is a complete set and therefore we can use it as a basis for the space and, in particular, we can write

$$|\psi_t\rangle = \sum_n a_n(t) e^{-\frac{i}{\hbar}\varepsilon_n t} |n\rangle$$
(11.40)

The reason for pulling out the phase factors will be clear shortly.

It is clear that if g = 0, then this is the correct general solution with

$$a_n(t) = a_n(0) = \text{constant}$$
(11.41)

The phase factors we pulled out represent the time dependence due to \hat{H}_0 and this is, by assumption, the major time dependence in the system.

If g is small we expect the time dependence of $a_n(t)$, which is due to the perturbation to be weak or that

$$\frac{da_n(t)}{dt} \text{ is small} \tag{11.42}$$

It is in this sense that we can propose to use perturbation theory on the system.

Using the eigenbasis expansion we have

$$\sum_{n} \left(i\hbar \frac{da_{n}(t)}{dt} + \varepsilon_{n} a_{n}(t) \right) e^{-\frac{i}{\hbar} \varepsilon_{n} t} |n\rangle$$
$$= \sum_{n} \left(\varepsilon_{n} a_{n}(t) + g \hat{U}_{t} a_{n}(t) \right) e^{-\frac{i}{\hbar} \varepsilon_{n} t} |n\rangle$$
(11.43)

Applying the linear functional $\langle m |$ from the left and using the orthonormality relation

$$\langle m \mid n \rangle = \delta_{mn} \tag{11.44}$$

we get

$$i\hbar \frac{da_m(t)}{dt} = g \sum_n \langle m | \hat{U}_t | n \rangle e^{i\omega_{mn}t} a_n(t)$$
$$= \sum_n V_{mn}(t) e^{i\omega_{mn}t} a_n(t)$$
(11.45)

where

$$\omega_{mn} = \frac{\varepsilon_m - \varepsilon_n}{\hbar} \tag{11.46}$$

This is an exact equation. It implies that the time dependence of $a_n(t)$ is due entirely to \hat{V}_t (because we explicitly extracted out the dependence due to \hat{H}_0). This is the interaction picture that we had earlier.

Exactly Solvable 2-State Example

Consider a 2-state system with

$$H_0 = \begin{pmatrix} E_1 & 0\\ 0 & E_2 \end{pmatrix} , \quad V(t) = \begin{pmatrix} 0 & \delta e^{i\omega t}\\ \delta e^{-i\omega t} & 0 \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}\\ V_{21} & V_{22} \end{pmatrix}$$
(11.47)

In the interaction picture, as derived above, we have

$$i\hbar \frac{dc_m(t)}{dt} = \sum_n V_{mn}(t)e^{i\omega_{mn}t}c_n(t) \quad , \quad |\psi_t\rangle = \sum_n c_n(t)e^{-\frac{i}{\hbar}\varepsilon_n t}|n\rangle \qquad (11.48)$$

or

$$i\hbar \frac{dc_1(t)}{dt} = \delta e^{i\left[\omega + \frac{E_1 - E_2}{\hbar}\right]t} c_2(t)$$
(11.49)

$$i\hbar \frac{dc_2(t)}{dt} = \delta e^{i\left[-\omega - \frac{E_1 - E_2}{\hbar}\right]t} c_1(t)$$
(11.50)

$$|\psi_t\rangle = c_1(t)e^{-\frac{i}{\hbar}E_1t}|1\rangle + c_2(t)e^{-\frac{i}{\hbar}E_2t}|2\rangle$$
(11.51)

We can write these equations as

$$\frac{dC(t)}{dt} = -\frac{i\delta}{\hbar} \begin{pmatrix} 0 & e^{i[\omega-\omega_{21}]t} \\ e^{-i[\omega-\omega_{21}]t} & 0 \end{pmatrix} C(t)$$
(11.52)

where

$$C(t) = \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} , \quad \omega_{21} = \frac{E_2 - E_1}{\hbar}$$
(11.53)

We can find an exact solution. With initial conditions $c_1(0) = 1$ and $c_2(0) = 0$ we get

$$|c_1(t)|^2 = \frac{\delta^2}{\delta^2 + \frac{\hbar^2(\omega - \omega_{21})^2}{4}} \sin^2 \Omega t = 1 - |c_2(t)|^2$$
(11.54)

where

$$\Omega^2 = \frac{\delta^2}{h^2} + \frac{(\omega - \omega_{21})^2}{4}$$
(11.55)

A graph of these functions is shown in Figure 11.1 below.



Figure 11.1: Exact Solution

A straightforward calculation gives

$$|c_1(t)|_{\min}^2 = \frac{(\omega - \omega_{21})^2}{(\omega - \omega_{21})^2 + \frac{4\delta^2}{\hbar^2}}$$
(11.56)

At resonance, $\omega = \omega_{21}$, we have

$$\Omega = \frac{\delta}{\hbar} \quad , \quad |c_1(t)|^2_{\min} = 0 \tag{11.57}$$

as shown in Figure 11.2 below.



Figure 11.2: At Resonance

The amplitude as a function of ω is shown in Figure 11.3 below.



Figure 11.3: Amplitude versus ω

where $\Delta = \text{full width at half maximum} = 4\delta/\hbar$. The amplitude is peaked at resonance and the width is proportional to δ (the strength of the perturbation).

This periodically forced 2–state system is a basic problem - it demonstrates the fundamental features of absorption and emission.

We now return to the full, general equations and look for a perturbation solution. Now we assume (power series)

$$a_n(t) = a_n^{(0)} + ga_n^{(1)} + g^2 a_n^{(2)} + \dots$$
(11.58)

Substituting and arranging the terms in a power series in g we have

$$\left(\frac{da_n^{(0)}}{dt}\right)g^0 + \left(i\hbar\frac{da_m^{(1)}}{dt} - \sum_n \langle m|\hat{U}_t|n\rangle e^{\frac{i}{\hbar}\omega_{mn}t}a_n^{(0)}\right)g^1 + \dots + \left(i\hbar\frac{da_m^{(r+1)}}{dt} - \sum_n \langle m|\hat{U}_t|n\rangle e^{\frac{i}{\hbar}\omega_{mn}t}a_n^{(r)}\right)g^r + \dots = 0$$

or looking at each order separately we have

$$0^{th} - \text{order} \quad \frac{da_n^{(0)}}{dt} = 0$$

$$1^{st} - \text{order} \quad i\hbar \frac{da_m^{(1)}}{dt} = \sum_n \langle m | \hat{U}_t | n \rangle e^{\frac{i}{\hbar}\omega_{mn}t} a_n^{(0)}$$

.....

$$(r+1)^{st} - \text{order} \quad i\hbar \frac{da_m^{(r+1)}}{dt} = \sum_n \langle m | \hat{U}_t | n \rangle e^{\frac{i}{\hbar}\omega_{mn}t} a_n^{(r)}$$

.....

Note that the coefficients $a_n^{(0)}$ follow from the initial condition

$$|\psi(0)\rangle = \sum_{n} a_n^{(0)} |n\rangle \tag{11.59}$$

The solution proceeds as follows:

initial condition
$$\rightarrow a_n^{(0)}$$

 $a_n^{(0)} \rightarrow a_n^{(1)}$ using the 1^{st} – order equation
......
 $a_n^{(r)} \rightarrow a_n^{(r+1)}$ using the $(r+1)^{st}$ – order equation

Now consider the following example. We assume that

$$\hat{H} = \hat{H}_0 \qquad t \le 0$$
 (11.60)

where

$$\hat{H}_0 |n\rangle = \varepsilon_n |n\rangle \tag{11.61}$$

and during the time interval $0 \le t \le T$ a perturbation \hat{V}_t is applied to the system and the $a_n(t)$ change with time.

Finally, for $t \ge T$ the perturbation is turned off and $a_n(t) = a_n(T)$.

.

The probability that, as a result of the perturbation, the energy of the system becomes ϵ_r , is given by

$$\left|\left\langle r \mid \psi_t \right\rangle\right|^2 = \left|\sum_i a_i(t) e^{-\frac{i}{\hbar}\varepsilon_i t} \left\langle r \mid i \right\rangle\right|^2 = \left|a_r(t)\right|^2 \tag{11.62}$$

and as $t \to \infty$ we get

$$\left|\left\langle r \mid \psi_t \right\rangle\right|^2 = \left|a_r(T)\right|^2 \tag{11.63}$$

Now to 1^{st} -order we have

$$i\hbar \frac{da_r^{(1)}}{dt} = \sum_n \langle r | \hat{U}_t | n \rangle e^{\frac{i}{\hbar}\omega_{rn}t} a_n^{(0)}$$
(11.64)

If $|\psi(0)\rangle = |i\rangle$, then

$$a_n^{(0)} = \begin{cases} 1 & n = i \\ 0 & n \neq i \end{cases}$$
(11.65)

This gives

$$i\hbar \frac{da_r^{(1)}}{dt} = \langle r | \hat{U}_t | i \rangle e^{\frac{i}{\hbar}\omega_{ri}t}$$
(11.66)

Integrating we have

$$a_r^{(1)}(T) = \frac{1}{i\hbar} \int_0^T \langle r | \hat{U}_t | i \rangle e^{\frac{i}{\hbar} (\varepsilon_r - \varepsilon_i) t} dt$$
(11.67)

and

$$a_r(T) = a_r^{(0)}(T) + ga_r^{(1)}(T)$$
(11.68)

which is identical to our earlier result as $t \to \infty$.

Now let return to our question. Has the state changed also?

In the example we found that the perturbation produces a final state $|\psi_t\rangle$ for $t \geq T$ which to $1^{st} \text{-} \text{order}$ is

$$|\psi_t\rangle = \sum_n a_n(t) e^{-\frac{i}{\hbar}\varepsilon_n t} |n\rangle$$
(11.69)

This is a coherent (definite relative phases) superposition of eigenvectors of \hat{H}_0 . This is *NOT* a stationary state. Interference effects between the terms in the sum are detectable. They do not, however, affect

$$|a_r(T)|^2$$
 = probability that the energy changes to ε_r (11.70)

Thus, the perturbation does not cause a *jump* from one stationary state $|i\rangle$ of \hat{H}_0 to another $|r\rangle$, but instead it produces a non-stationary state.

The conventional language of quantum mechanics produces this ambiguity between the two statements

the energy is
$$\epsilon_r$$
 and the state is $|r\rangle$

For the state

$$\left|\psi_{t}\right\rangle = \sum_{n} a_{n}(t) e^{-\frac{i}{\hbar}\varepsilon_{n}t} \left|n\right\rangle$$

it is correct to say

the probability of the energy being ϵ_r is $|a_r(T)|^2$

or

$$Prob(E = \epsilon_r ||\psi\rangle) = |a_r(T)|^2$$

The state, however, is $|\psi_t\rangle$ and NOT $|r\rangle$.

An example

Suppose we perturb an oscillator with a decaying electric field of the form

$$\hat{V}_t = -q\mathcal{E}_0 \hat{x} e^{-\frac{t}{\tau}} \qquad t \ge 0$$
 (11.71)

To 1^{st} -order, starting with the initial state $|n\rangle$ with energy

$$\varepsilon_n = \hbar\omega(n + \frac{1}{2}) \tag{11.72}$$

we have

$$|\psi(t)\rangle = |n\rangle + \frac{1}{i\hbar} \int_{0}^{t} dt' \hat{V}(t) |n\rangle \qquad (11.73)$$

where

$$\hat{V}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t} \hat{V}_t e^{-\frac{i}{\hbar}\hat{H}_0 t}$$
(11.74)

We let n = 0 (the ground state) for this example. We then have

$$|\psi(t)\rangle = |0\rangle + \frac{1}{i\hbar} \int_{0}^{t} dt' e^{\frac{i}{\hbar}\hat{H}_{0}t} (-q\mathcal{E}_{0}\hat{x}) e^{-\frac{t}{\tau}} e^{-\frac{i}{\hbar}\hat{H}_{0}t} |0\rangle$$
(11.75)

Using

$$e^{-\frac{i}{\hbar}\hat{H}_{0}t}\left|0\right\rangle = e^{-i\frac{\omega}{2}t}\left|0\right\rangle \tag{11.76}$$

$$\hat{x}\left|0\right\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left|1\right\rangle \tag{11.77}$$

$$e^{\frac{i}{\hbar}\hat{H}_0t}\left|1\right\rangle = e^{i\frac{3\omega}{2}t}\left|0\right\rangle \tag{11.78}$$

we get (letting $t \to \infty$)

$$|\psi(t)\rangle = |0\rangle + \frac{1}{i\hbar}(-q\mathcal{E}_0)\sqrt{\frac{\hbar}{2m\omega}}\int_0^\infty dt' e^{i\omega t' - \frac{t}{\tau}}|1\rangle$$
(11.79)

and finally,

$$P_{0\to 1} = |\langle 1 | \psi(t) \rangle|^{2} = \frac{q^{2} \mathcal{E}_{0}^{2}}{2m\hbar\omega} \left| \int_{0}^{\infty} dt' e^{i\omega t' - \frac{t}{\tau}} \right|^{2}$$
$$= \frac{q^{2} \mathcal{E}_{0}^{2}}{2m\hbar\omega} \frac{\tau^{2}}{\tau^{2}\omega^{2} + 1}$$
(11.80)

We now return to the earlier general result (11.36) we derived for the probability, namely, $\Delta t = 2$

$$P_{0 \to n}(t) = \left| \langle n | \hat{V}_{t'} | 0 \rangle \right|^2 \left(\frac{\sin \frac{\Delta t}{2\hbar}}{\Delta/2} \right)^2 \tag{11.81}$$

In Figure 11.4 below we plot this function.



Figure 11.4: Probability(0,n) versus Delta

The height of the central peak is proportional to t^2 and the location of the first zero is at

$$\Delta = \frac{2\pi\hbar}{t} \tag{11.82}$$

so that the width of the peak decreases as 1/t.

The formula implies that for very short times

$$P_{0 \to n} \propto t^2 \text{ for all } \varepsilon_n$$
 (11.83)

As $t \to \infty$, however, the probability is largest for those states whose energy lies under the sharp bump near $\Delta = 0$ or those states with whose energy lies under the peak around ϵ_0 . Now the energy $\epsilon_n \approx \epsilon_0$ lies under the sharp bump when

$$|\Delta| = |\varepsilon_n - \varepsilon_0| < \frac{2\pi\hbar}{t} \tag{11.84}$$

The area under the bump is proportional to t and the rest of the area oscillates in time around zero. This latter feature means that if $\epsilon_n \neq \epsilon_0$, the transition probability oscillates in time with a repetition time of

$$\frac{2\pi\hbar}{|\varepsilon_n - \varepsilon_0|} \tag{11.85}$$

The case, where we are looking for a transition to a single state, is, thus, only valid in perturbation theory for very small time t. Otherwise the condition that the

$$P_{0\to0}(t) \approx 1 \tag{11.86}$$

will not be true and perturbation theory breaks down. We also note that the probability cannot grow larger than one or that, after a while, the higher-order effects of the perturbation which we have neglected so far must become important and prevent the probability from exceeding one.

The condition that tells us whether a transition probability to a state with an energy appreciably different than the original energy is the same condition in time-independent perturbation theory that tells whether the state vector changes appreciably from the unperturbed state, namely

$$\left|\frac{\langle n|\tilde{V}|0\rangle}{\varepsilon_n - \varepsilon_0}\right| << 1 \tag{11.87}$$

Physically, a more interesting case occurs when the state $|n\rangle$ is one of a continuum of energy states, or it lies in a group of very closely spaced levels.

In this case we ask a different experimental question, namely,

What is the probability that the system makes

- a transition to a small group of states near
- $|n\rangle$ (or has energy near ϵ_n)?

Since the area under the bump near $\Delta = 0$ or $\epsilon_n \approx \epsilon_0$ is proportional to t, we expect that the transition probability to a small group of states near ϵ_0 will grow linearly with t and thus

$$\frac{P_{0 \to n}(t)}{t} = \text{ transition rate } = \Gamma = \text{ constant as } t \to \infty$$
 (11.88)

Quantities that we measure are related to the transition rate and this result says that these measurements will make sense.

Let us now carry out this derivation in detail.

To calculate this transition rate we must sum $P_{0\to n}$ over the group of *final* states. We assume that $|\langle b| \hat{V}_{t'} |0\rangle|^2$ is relatively constant over the small group of states near $|n\rangle$ (has a weak energy dependence).

We then have

$$\sum_{\substack{n \\ ingroup}} P_{0 \to n}(t) = \left| \langle n | \hat{V}_{t'} | 0 \rangle \right|^2 \int_{group} d\varepsilon_n \rho(\varepsilon_n) \left[\frac{\sin\left[\frac{(\varepsilon_n - \varepsilon_0)t}{h}\right]}{\left[\frac{(\varepsilon_n - \varepsilon_0)}{2}\right]} \right]^2$$
(11.89)

where

 $\rho(\varepsilon_n) = \text{number of states per unit energy}$ $\rho(\varepsilon_n)d\varepsilon_n = \text{number of states in the interval } d\varepsilon_n$ Now in the limit $t \to \infty$

$$\left[\frac{\sin\left[\frac{(\varepsilon_n-\varepsilon_0)t}{\hbar}\right]}{\left[\frac{(\varepsilon_n-\varepsilon_0)}{2}\right]}\right]^2 \to \frac{2\pi t}{\hbar}\delta(\varepsilon_0-\varepsilon_n)$$
(11.90)

i.e., in general, for a sequence of functions

$$\delta_t(\alpha) = \frac{\sin^2 \alpha t}{\pi \alpha^2 t} \tag{11.91}$$

we have that

$$\delta_t(\alpha) = \begin{cases} \frac{t}{\pi} & \alpha = 0\\ \leq \frac{1}{\pi\alpha^2 t} & \alpha \neq 0 \end{cases}$$
(11.92)

and

$$\lim_{t \to \infty} \int_{-\infty}^{\infty} d\alpha \delta_t(\alpha) F(\alpha) = F(0)$$
(11.93)

Therefore,

$$\lim_{t \to \infty} \delta_t(\alpha) = \delta(\alpha) \tag{11.94}$$

Using this result, we have

$$\sum_{n} P_{0 \to n}(t) = \Gamma t \tag{11.95}$$

and thus

$$\Gamma = \text{ transition rate } = \frac{2\pi}{\hbar} \left| \langle n | \hat{V} | 0 \rangle \right|^2 \rho(\varepsilon_n)_{\varepsilon_n = \varepsilon_0}$$
(11.96)

which is called *Fermi's Golden Rule*.

We now consider a perturbation that depends explicitly on time. In particular, suppose we have a harmonic perturbation of the form

$$\hat{V}_t = \hat{V}e^{\eta t}\cos\omega t = \frac{\hat{V}}{2}e^{\eta t}\left(e^{-i\omega t} + e^{i\omega t}\right)$$
(11.97)

and $|\psi(t_0)\rangle = |0\rangle$, where we let $t_0 \to -\infty$. The $e^{\eta t}$ factor is necessary to make the mathematical operations valid in the limit. It is equivalent for small η to turning the perturbation on slowly. In the end we will let $\eta \to 0$.

We have

$$\langle n \mid \psi(t) \rangle = \langle n \mid 0 \rangle + \frac{1}{i\hbar} e^{-\frac{i}{\hbar}\varepsilon_n t} \int_{-\infty}^{0} dt' \langle n | \hat{V}(t') | 0 \rangle$$

$$= \frac{e^{\eta t}}{2} \left[\frac{e^{i(\varepsilon_n - \varepsilon_0 - \hbar\omega)\frac{t}{\hbar}}}{\varepsilon_0 - \varepsilon_n + \hbar\omega + i\hbar\eta} + \frac{e^{i(\varepsilon_n - \varepsilon_0 + \hbar\omega)\frac{t}{\hbar}}}{\varepsilon_0 - \varepsilon_n - \hbar\omega + i\hbar\eta} \right] \langle n | \hat{V} | 0 \rangle$$

$$(11.98)$$

Thus, the probability of the energy being ϵ_n at the time t is

$$\left| \langle n \mid \psi(t) \rangle \right|^{2} = \frac{e^{2\eta t}}{4} \left| \langle n \mid \hat{V} \mid 0 \rangle \right|^{2} \left\{ \begin{array}{c} \frac{1}{(\varepsilon_{0} - \varepsilon_{n} + \hbar\omega)^{2} + (\hbar\eta)^{2}} + \frac{1}{(\varepsilon_{0} - \varepsilon_{n} - \hbar\omega)^{2} + (\hbar\eta)^{2}} \\ + 2\operatorname{Re} \frac{e^{-2i\omega t}}{(\varepsilon_{0} - \varepsilon_{n} + \hbar\omega + i\hbar\eta)(\varepsilon_{0} - \varepsilon_{n} - \hbar\omega + i\hbar\eta)} \end{array} \right\}$$
(11.99)

The first term comes from the $e^{-i\omega t}$ part of \hat{V}_t (positive frequency) and the second term comes from the $e^{i\omega t}$ part of \hat{V}_t (negative frequency). The last term represents *interference effects*.

Since

$$P_{0 \to n}(t) = \Gamma_{0 \to n} t \tag{11.100}$$

we have

$$\Gamma_{0 \to n} = \frac{dP_{0 \to n}(t)}{dt} \tag{11.101}$$

and thus

$$\Gamma_{0 \to n} \tag{11.102}$$

$$= \frac{e^{2\eta t}}{4} \left| \langle n | \hat{V} | 0 \rangle \right|^2 \left\{ \begin{array}{c} \left[\frac{1}{(\varepsilon_0 - \varepsilon_n + \hbar\omega)^2 + (\hbar\eta)^2} + \frac{1}{(\varepsilon_0 - \varepsilon_n - \hbar\omega)^2 + (\hbar\eta)^2} \right] (1 - \cos 2\omega t) \\ + 2\sin 2\omega t \left[\frac{e^{-2i\omega t}}{(\varepsilon_0 - \varepsilon_n + \hbar\omega + i\hbar\eta)(\varepsilon_0 - \varepsilon_n - \hbar\omega + i\hbar\eta)} \right] \end{array} \right\}$$

The $\sin \omega t$ and $\cos \omega t$ terms arise from the interference term. In the limit $\eta \to 0$ and assuming that $|n\rangle$ is in the continuum part of spectrum, we have

- 1. the first two terms are not equal to zero only if $\varepsilon_n-\varepsilon_0=\pm\hbar\omega$
- 2. the $\sin \omega t$ and $\cos \omega t$ terms average to zero if we assume that $\Gamma_{0\to n}$ is $dP_{0\to n}(t)/dt$ averaged over a few cycles of \hat{V}_t

which gives the result

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar} \frac{\left|\langle n|\hat{V}|0\rangle\right|^2}{4} \left[\delta(\varepsilon_n - \varepsilon_0 - \hbar\omega) + \delta(\varepsilon_n - \varepsilon_0 + \hbar\omega)\right]$$
(11.103)

The positive and negative frequency parts act independently and the interference averages to zero.

Thus, the $e^{-i\omega t}$ part produced a $\Delta E > 0$ process (absorption), while the $e^{i\omega t}$ part produced a $\Delta E < 0$ process (emission).

To enhance our understanding of time-dependent perturbation theory, we look at a variation of this harmonic perturbation. Suppose we have a harmonic perturbation of the form

$$\hat{V}_{t} = \hat{V}e^{-i\omega t} + \hat{V}^{+}e^{i\omega t}$$
(11.104)

which is only applied for a finite time interval $0 \le t \le T$. If we start with energy ϵ_i in the state $|i\rangle$, then at any time $t \ge T$

$$\begin{aligned} a_f^{(1)}(t) &= 1^{st} - \text{order amplitude for the state } |\psi(t)\rangle \\ & \text{to have energy } \varepsilon_f \text{ (be in state } |f\rangle?) \quad f \neq i \end{aligned}$$

is given by

$$a_{f}^{(1)}(T) = \frac{1}{i\hbar} \langle f | \hat{V} | i \rangle \int_{0}^{T} e^{i(\omega_{fi} - \omega)t} dt + \frac{1}{i\hbar} \langle f | \hat{V}^{+} | i \rangle \int_{0}^{T} e^{i(\omega_{fi} + \omega)t} dt \qquad (11.105)$$

and

$$a_f^{(1)}(T)\Big|^2$$
 = probability that the final energy will be ϵ_f (11.106)

As an example we consider spin resonance (we solved this problem exactly earlier).

We consider a spin = 1/2 particle in a static magnetic field B_0 (in the z-direction). This says that the unperturbed Hamiltonian is

$$\hat{H}_0 = -\frac{1}{2}\hbar\gamma B_0\hat{\sigma}_z \tag{11.107}$$

This operator has the eigenvectors and eigenvalues

$$|+\rangle = \begin{pmatrix} 1\\0 \end{pmatrix}, \ |-\rangle = \begin{pmatrix} 0\\1 \end{pmatrix}, \quad \epsilon_{\pm} = \pm \frac{1}{2}\hbar\gamma B_0 \qquad (11.108)$$

We now perturb the system with another magnetic field B_1 , which is rotating in the x - y plane with angular velocity ω . This implies that

$$\hat{V}_{t} = -\frac{1}{2}\hbar\gamma B_{1}(\cos\omega t\hat{i} + \sin\omega t\hat{j})\cdot\hat{\sigma}$$

$$= -\frac{1}{2}\hbar\gamma B_{1}\left[\hat{\sigma}_{x}\cos\omega t + \hat{\sigma}_{y}\sin\omega t\right] = -\frac{1}{2}\hbar\gamma B_{1}\begin{pmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{pmatrix}$$

$$= -\frac{1}{2}\hbar\gamma B_{1}\left(\hat{V}e^{-i\omega t} + \hat{V}^{+}e^{i\omega t}\right)$$
(11.109)

where

$$\hat{V} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} , \quad \hat{V}^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$
(11.110)

We choose the initial state to be

$$|i\rangle = |n\rangle$$
 (spin up in the z-direction) (11.111)

The first order perturbation theory approximation for this result is

$$\left|a_{f}^{(1)}(T)\right|^{2} = \left(\frac{\omega_{1}}{\omega_{0}+\omega}\right)^{2} \sin^{2}\frac{1}{2}(\omega_{0}+\omega)T$$
 (11.112)

where

$$\omega_0 = \gamma B_0 \quad , \quad \omega_1 = \gamma B_1 \tag{11.113}$$

and we have used

$$\langle -|\hat{V}|+\rangle = 0, \ \langle -|\hat{V}^{+}|+\rangle = -\frac{1}{2}\hbar\gamma B_{1}$$
 (11.114)

$$\omega_{fi} = \frac{\varepsilon_f - \varepsilon_i}{\hbar} = \omega_0 \tag{11.115}$$

When is the first order perturbation theory result valid?

If we compare the exact result with perturbation theory by expanding the exact result in a power series, we find that the two results agree exactly if

$$\left|\frac{\omega_1}{\omega_0 + \omega}\right| << 1 \tag{11.116}$$

which corresponds $B_1 \ll B_0$ (as long as $\omega_0 + \omega \neq 0$). When $\omega_0 + \omega = 0$ we have a phenomenon called resonance. The exact solution gives

$$|a_f(T)|^2 = \sin^2 \frac{1}{2}\alpha T$$
 (11.117)

where $\alpha^2 = (\omega_0 + \omega)^2 + \omega_1^2$ and perturbation theory gives

$$\left|a_{f}^{(1)}(T)\right|^{2} = \left(\frac{\omega_{1}T}{2}\right)^{2}$$
(11.118)

Thus, the results agree only if $|\omega_1 T| \ll 1$ or if the perturbation only acts for a short time.

11.2 Atomic Radiation and Selection Rules

We now apply time-independent perturbation theory to the absorption and emission electromagnetic radiation by matter.

The Hamiltonian for an electron in an atom interacting with and electromagnetic field is

$$\hat{H} = \frac{\left(\vec{p}_{op} - \frac{q}{c}\vec{A}\right)^2}{2m_e} + q\phi + U$$
(11.119)

where q = -e, U = the potential energy function that binds the electrons in the atom, and \vec{A} and φ are the vector and scalar potentials associated with the electromagnetic field.

These potentials imply the electric and magnetic fields

$$\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t}, \vec{B} = \nabla \times \vec{A}$$
(11.120)

Note that if $\vec{A} = 0$, the $\vec{B} = 0$ and

$$\phi = -\int_{0}^{\vec{r}} \vec{E}(\vec{r},t) \cdot d\vec{r} \qquad (11.121)$$

We rewrite \hat{H} as

$$\hat{H} = \hat{H}_0 + \hat{V}$$
(11.122)

where

$$\hat{H}_0 = \frac{\vec{p}_{op}^2}{2m_e} + U = \text{Hamiltonian for the atom with no electromagnetic field}$$
(11.123)

and

$$\hat{V} = \frac{q}{2m_e c} \left(\vec{p}_{op} \cdot \vec{A} + \vec{A} \cdot \vec{p}_{op} \right) + \frac{q^2}{2m_e c^2} \left(\vec{A} \cdot \vec{A} \right) + q\phi$$
(11.124)

is the perturbation due to the presence of the electromagnetic field, i.e., the term \hat{V} tells us how the atom interacts with the electromagnetic field.

11.2.1 The Electric Dipole Approximation

The typical wavelength of visible electromagnetic radiation is ≈ 5000 and the typical dimension of an atom is \approx a few . This implies that the electromagnetic fields are approximately constant over the volume of the atom.

In Gaussian units $|\vec{E}| \approx |\vec{B}|$, but the force due to $\vec{B} \approx (v/c) \times$ the force due to \vec{E} . Thus, magnetic effects are negligible in most atoms compared to electric effects. We therefore assume

- 1. $\vec{E}\approx$ constant over the volume of the atom
- 2. \vec{B} can be neglected

This is the so-called electric dipole approximation.

In this approximation, we have $\vec{A} = 0$ and as we said above (11.121), $\vec{B} = 0$ and

$$\phi = -\int_{0}^{\vec{r}} \vec{E}(\vec{r},t) \cdot d\vec{r} \qquad (11.125)$$

This last integral is independent of path since

$$\nabla \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0 \tag{11.126}$$

Since we are assuming that $\vec{E} \approx \text{constant}$ over the volume of the atom, we get

$$\phi = -\vec{r} \cdot \vec{E}(t) \tag{11.127}$$

This adds a perturbation of the form

$$\hat{V} = -q\vec{r}\cdot\vec{E}(t) \tag{11.128}$$

to the Hamiltonian.

In some derivations the quantity

$$\hat{V} = \frac{q}{2m_e c} \left(\vec{p}_{op} \cdot \vec{A} + \vec{A} \cdot \vec{p}_{op} \right) + \frac{q^2}{2m_e c^2} \left(\vec{A} \cdot \vec{A} \right) + q\phi$$
(11.129)

is chosen as the perturbation. The next step would be to expand in powers of the potentials. Since $\nabla \cdot \vec{E} = 0$ for the radiation field, we can choose $\varphi = 0$ and $\nabla \cdot \vec{A} = 0$ (if these relations were not true we could make them so with a gauge transformation).

Therefore, we end up with an expansion in powers of \vec{A} . The first term in the expansion is

$$\hat{V}_{Ap} = -\frac{q}{2m_e c} \left(\vec{p}_{op} \cdot \vec{A} + \vec{A} \cdot \vec{p}_{op} \right) = -\frac{q}{m_e c} \vec{A} \cdot \vec{p}_{op}$$
(11.130)

since

$$\vec{p}_{op} \cdot \vec{A} - \vec{A} \cdot \vec{p}_{op} \propto \nabla \cdot \vec{A} = 0$$
(11.131)

In this case, in the electric dipole approximation

$$\vec{E} \approx \text{ constant}$$
 , $\vec{B} = 0$
 $\vec{A}(\vec{r},t) = -c \int_{0}^{\vec{r}} \vec{E}(\vec{r},t) dt$
 $\phi(\vec{r},t) = 0$

If $\vec{E}(\vec{r},t) = \vec{E}(\vec{r})e^{-i\omega t}$, then $\vec{A} = e\vec{E}/i\omega$. Using

$$\frac{\vec{p}_{op}}{m} = \frac{i}{\hbar} \left[\hat{H}_0, \vec{r}_{op} \right] \tag{11.132}$$

we get

$$\hat{V}_{Ap} = -\frac{q}{\hbar\omega} \left[\hat{H}_0, \vec{r}_{op} \right] \cdot \vec{E}$$
(11.133)

We can then calculate matrix elements

$$\langle m | \hat{V}_{Ap} | n \rangle = -\frac{q}{\hbar\omega} \langle m | \hat{H}_0 \vec{r}_{op} - \vec{r}_{op} \hat{H}_0 | n \rangle \cdot \vec{E}$$

$$= -\frac{q}{\hbar\omega} (\varepsilon_m - \varepsilon_n) \langle m | \vec{r}_{op} \cdot \vec{E} | n \rangle$$

$$= \frac{\omega_{mn}}{\omega} \langle m | \hat{V} | n \rangle$$
(11.134)

where

$$\omega_{mn} = \frac{\varepsilon_m - \varepsilon_n}{\hbar} \tag{11.135}$$

Thus, the matrix elements of \hat{V}_{Ap} (from $\hat{A} \cdot \vec{p}_{op}$) differ from the matrix elements of \hat{V} (from φ) by the factor ω_{mn}/ω . This implies different transition probabilities in first order except at resonance where $\omega_{mn}/\omega = 1$. The reason for the differences is as follows:

- 1. we assumed that the perturbation = 0 for $t \leq 0\,,\, t \geq T$
- 2. there is no physical problem with $V = -q\vec{r} \cdot \vec{E}$ changing discontinuously
- 3. however, if $\vec{A} \cdot \vec{p}_{op}$ changes discontinuously, then the relation

$$\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t} \tag{11.136}$$

generates spurious δ -function type \vec{E} fields

It is clear that one must exercise great care in choosing a starting point for perturbation theory.

11.2.2 Induced Emission and Absorption

We now look at the physics connected with the harmonic perturbation. Physically, it represents an electromagnetic wave interacting with the atom.

We consider the perturbing potential

$$\hat{V} = \begin{cases} -q\vec{r} \cdot \vec{E}_0 (e^{-i\omega t} + e^{i\omega t}) & 0 < t < T \\ 0 & t < 0, t > T \end{cases}$$
(11.137)

where \vec{E}_0 = a constant vector which tells us the strength and polarization of the electromagnetic field.

This perturbing potential corresponds to monochromatic(single wavelength) electromagnetic radiation.

For an initial state $|\psi(0)\rangle = |i\rangle$ where $\hat{H}_0 |i\rangle = \epsilon_i |i\rangle$ the probability, at any time $t \ge T$, that the atom will have a final energy ϵ_f is

$$P_{i \to f}(T) = \left| a_f^{(1)}(T) \right|^2 \tag{11.138}$$

to first order, where we have from our earlier derivation

$$a_f^{(1)}(T) = \frac{\langle f | \left(-q\vec{r} \cdot \vec{E}_0 \right) | i \rangle}{\hbar} \left[\frac{1 - e^{i(\omega_{fi} - \omega)T}}{\omega_{fi} - \omega} + \frac{1 - e^{i(\omega_{fi} + \omega)T}}{\omega_{fi} + \omega} \right]$$
(11.139)

If $\epsilon_f > \epsilon_i$ this gives the probability amplitude for absorbing radiation and if $\epsilon_f < \epsilon_i$ this gives the probability amplitude for emitting radiation.

In the limit $T \to \infty$, as we saw earlier, $P_{i \to f}(t) = \Gamma_{i \to f} t$ which gives

$$\Gamma_{i \to f} = \frac{2\pi q^2}{\hbar} \frac{\left| \langle f | \vec{r} \cdot \vec{E}_0 | i \rangle \right|^2}{4} \left[\delta(\varepsilon_i - \varepsilon_f - \hbar\omega) + \delta(\varepsilon_i - \varepsilon_f + \hbar\omega) \right]$$
(11.140)

In this expression

$$\delta(\varepsilon_i - \varepsilon_f - \hbar\omega) \to \text{ absorption}$$

$$\delta(\varepsilon_i - \varepsilon_f + \hbar\omega) \to \text{ emission}$$

We then have the transition rates

$$\Gamma^{a}_{i \to f} = \Gamma^{e}_{i \to f} = \frac{2\pi q^2}{\hbar} \frac{\left| \langle f | \vec{r} \cdot \vec{E}_0 | i \rangle \right|^2}{4}$$
(11.141)

These expressions are *zero/nonzero* or transitions are *not-allowed/allowed* depending on the matrix element of the perturbation, i.e.,

if for $i \to f \quad \langle f | \vec{r} \cdot \vec{E}_0 | i \rangle = 0$, then the transition $i \to f$ is not allowed

These relationships between the quantum numbers of the initial and final states that tell us whether or not a transition is allowed are called *selection rules*.

To determine the selection rules for one-electron atoms we only need to consider matrix elements of the form

$$\langle n'\ell' m_{\ell'} m_{s'} | \vec{r} \cdot \vec{E}_0 | n\ell m_\ell m_s \rangle \tag{11.142}$$

or we need to look at three matrix elements, namely,

$$\langle n'\ell'm_{\ell'}m_{s'}|\hat{x}|n\ell m_{\ell}m_s\rangle, \langle n'\ell'm_{\ell'}m_{s'}|\hat{y}|n\ell m_{\ell}m_s\rangle \text{ and } \langle n'\ell'm_{\ell'}m_{s'}|\hat{z}|n\ell m_{\ell}m_s\rangle$$

Now

$$z = r\cos\theta \propto rY_{10} = x_3 \tag{11.143}$$

$$x = r\sin\theta\cos\varphi \propto r(Y_{11} + Y_{1,-1}) = x_1 \tag{11.144}$$

$$y = r\sin\theta\sin\varphi \propto r(Y_{11} - Y_{1,-1}) = x_2 \tag{11.145}$$

A typical matrix element, therefore, will have a term like the following:

$$\langle sm_{s'} | sm_s \rangle \int R_{n'\ell'}(r) R_{n\ell}(r) r^3 dr \int Y^*_{\ell'm\ell'} Y_{\ell m_\ell} Y_{1m} d\Omega \qquad (11.146)$$

where $m = \pm 1, 0$.

The radial integral would equal zero only by accident implying that it is not part of the general selection rules, which must come from the other terms.
The term $\langle sm_{s'} | sm_s \rangle = \delta_{m_{s'}m_s}$ gives us a simple selection rule (this simple rule arises here because the interaction does not depend on spin). We have

$$m_{s'} = m_s \rightarrow \text{ the } \Delta m_s = 0$$
 SELECTION RULE (11.147)

The rest of the selection rules come from the angular integration terms

$$\int Y_{\ell'm_{\ell'}}^* Y_{\ell m_{\ell}} Y_{1m} d\Omega \tag{11.148}$$

This integral equals 0 unless $\ell + \ell' + 1 =$ an even integer. This rule follows from parity considerations. For any angular integration over all angles to be nonzero, the integrand must be even under the parity operation.

Now

$$Y_{\ell m} \to (-1)^{\ell} Y_{\ell m} \tag{11.149}$$

under the parity operation. Therefore

$$Y_{\ell'm\ell'}^* Y_{\ell m\ell} Y_{1m} \to (-1)^{\ell+\ell'+1} Y_{\ell'm\ell'}^* Y_{\ell m\ell} Y_{1m}$$
(11.150)

which gives the stated rule.

The θ -integration says that we must have

$$|\ell' - \ell| \le 1 \le \ell' + \ell$$

This corresponds to thinking of the integrand as made up of two states, namely,

$$\langle \ell' m_{\ell'} | (|\ell m_{\ell}\rangle \otimes |1m\rangle)$$

Our angular momentum addition rules say that

$$|\ell m_{\ell}\rangle \otimes |1m\rangle = |\ell+1\rangle \oplus |\ell\rangle \oplus |\ell-1\rangle$$

and the selection rule then follows from the orthogonality condition.

The two ℓ -rules when combined imply the selection rule

$$\Delta m_{\ell} = m_{\ell'} - m_{\ell} = \pm 1,0 \qquad \text{SELECTION RULE} \tag{11.151}$$

Thus, for transitions within the electric dipole approximation, as defined above, we have the SELECTION RULES

$$\Delta m_{\ell} = m_{\ell'} - m_{\ell} = \pm 1, 0 \tag{11.152}$$
$$\Delta \ell = \ell' - \ell = \pm 1 \tag{11.153}$$

$$\Delta \ell = \ell' - \ell = \pm 1 \tag{11.153}$$

$$\Delta m_s = 0 = \Delta s \tag{11.154}$$

The derivation is more complex for multi-electron atoms due the complexity of the wave function (see next chapter), but it can be shown that, in general, the SELECTION RULES in the electric dipole approximation are

- 1. parity changes
- 2. $\Delta(\sum \ell_i) = \pm 1$
- 3. $\Delta S = 0$
- 4. $\Delta M_S = 0$
- 5. $\Delta L = \pm 1,0$ (possibility of 0 which is not allowed for 1-electron atoms)
- 6. $\Delta M_L = \pm 1, 0$
- 7. $\Delta J = \pm 1, 0$
- 8. $\Delta M_J = \pm 1, 0$
- 9. $J = 0 \rightarrow J = 0$ is strictly forbidden

11.3 A Real Physical Process - Ionization

We now carry out the calculations of the transition rate for the ionization(transition to the continuum) of hydrogen by electromagnetic radiation.

The initial state of the electron is the ground state of hydrogen

$$|i\rangle = |100\rangle$$
 with energy $\varepsilon_i = \varepsilon_{100} = -\frac{e^2}{2a_0}$ (11.155)

The final state of the electron in the ionization process is a free particle state(ionized electron)

$$|f\rangle = \left|\vec{k}\right\rangle$$
 with energy $\varepsilon_f = \varepsilon_k = \frac{\hbar^2 k^2}{2m}$ (11.156)

We then have

$$\vec{p}_{op}\left|\vec{k}\right\rangle = \hbar\vec{k}\left|\vec{k}\right\rangle \tag{11.157}$$

which says this is a momentum eigenstate also (for free particles $[\hat{H}, \vec{p}_{op}] = 0$ and momentum and energy have the same eigenstates). The momentum is given by $\vec{p} = \hbar \vec{k}$. Since $\varepsilon_f > \varepsilon_i$ this is an absorption process and thus the transition rate is given by

$$\Gamma_{0 \to \vec{k}} = \text{transition} \text{rate} = \lim_{t \to \infty} \frac{P_{0 \to \vec{k}}(t)}{t}$$
$$= \frac{2\pi}{\hbar} \left| \left\langle \vec{k} \right| \hat{V} \left| 100 \right\rangle \right|^2 \delta(\varepsilon_k - \varepsilon_{100} - \hbar\omega)$$
(11.158)

where ω = frequency of the electromagnetic radiation and

 \hat{V} = $-e\vec{r}\cdot\vec{\mathcal{E}}$ (electric dipole approximation)

 $\vec{\mathcal{E}}$ = the electric field vector

We define

$$d\Gamma = \text{ rate of transition into a small solid angle } d\Omega$$
$$= \sum_{\vec{k} \text{ in } d\Omega} \Gamma_{0 \to \vec{k}}$$
(11.159)

For convenience we use a common trick and assume that the universe is a large box (side = L, volume = L^3). This allows us to normalize the plane wave states associated with the free electron. We have

$$\langle \vec{r} \mid \vec{k} \rangle = A e^{i \vec{k} \cdot \vec{r}}$$

$$\langle \vec{k} \mid \vec{k} \rangle = 1 = \int d^3 \vec{r} \langle \vec{k} \mid \vec{r} \rangle \langle \vec{r} \mid \vec{k} \rangle$$

$$(11.160)$$

$$\kappa_{j} = 1 = \int d^{3}\vec{r} \, e^{-i\vec{k}\cdot\vec{r}} e^{i\vec{k}\cdot\vec{r}} = A^{2} \int d^{3}\vec{r} = A^{2}L^{3}$$
(11.161)

or

$$A = \frac{1}{L^{3/2}} \tag{11.162}$$

Now there are

$$L^{3} \frac{d^{3} \vec{k}}{(2\pi)^{3}} = \frac{L^{3}}{(2\pi)^{3}} d\Omega k^{2} dk = \frac{L^{3} m k}{(2\pi)^{3} \hbar^{2}} d\Omega d\varepsilon_{k}$$
(11.163)

states in the volume $d^3\vec{k}$ of phase space. This implies that there are

$$\frac{L^3 mk}{(2\pi)^3 \hbar^2} \tag{11.164}$$

states per unit energy per unit solid angle.

Therefore,

$$d\Gamma = \sum_{\vec{k} \text{ in } d\Omega} \Gamma_{0 \to \vec{k}} \to d\Omega \int_{0}^{\infty} \frac{L^{3} m k}{(2\pi)^{3} \hbar^{2}} d\varepsilon_{k} \frac{\pi e^{2}}{2\hbar} \left| \left\langle \vec{k} \right| \vec{r} \cdot \vec{\mathcal{E}} \left| 100 \right\rangle \right|^{2} \delta(\varepsilon_{k} - \varepsilon_{100} - \hbar\omega)$$

Doing the integration (using the delta function) we get

$$d\Gamma = d\Omega \frac{L^3 m k e^2}{16\pi^2 \hbar^3} \left| \left\langle \vec{k} \right| \vec{r} \cdot \vec{\mathcal{E}} \left| 100 \right\rangle \right|^2 \tag{11.165}$$

where

$$\varepsilon_k = \varepsilon_{100} + \hbar\omega = \frac{\hbar^2 k^2}{2m} \tag{11.166}$$

$$k = \left(\frac{2m\omega}{\hbar} - \frac{1}{a_0^2}\right)^{1/2} \tag{11.167}$$

11.3.1 Evaluation of the Matrix Element

We have

$$\langle \vec{k} | \vec{r} \cdot \vec{\mathcal{E}} | 100 \rangle = \int d^{3}\vec{r} \langle \vec{k} | \vec{r} \rangle \langle \vec{r} | \vec{r} \cdot \vec{\mathcal{E}} | 100 \rangle$$

$$= \frac{1}{L^{3/2}} \int d^{3}\vec{r} e^{-i\vec{k}\cdot\vec{r}} \vec{r} \cdot \vec{\mathcal{E}} \langle \vec{r} | 100 \rangle$$

$$= \frac{1}{L^{3/2}} \int d^{3}\vec{r} e^{-i\vec{k}\cdot\vec{r}} \vec{r} \cdot \vec{\mathcal{E}} R_{10}(r) Y_{00}$$

$$= \frac{2}{a_{0}^{3/2} L^{3/2}} \int d^{3}\vec{r} e^{-i\vec{k}\cdot\vec{r}} e^{-\frac{r}{a_{0}}} \vec{r} \cdot \vec{\mathcal{E}}$$
(11.168)

We can arbitrarily choose $\vec{k} = k\hat{z}$ which gives

$$\left\langle \vec{k} \middle| \vec{r} \cdot \vec{\mathcal{E}} \middle| 100 \right\rangle = \frac{2}{a_0^{3/2} L^{3/2}} \int d\Omega dr r^2 e^{-ikr\cos\theta - \frac{r}{a_0}} \vec{r} \cdot \vec{\mathcal{E}}$$
(11.169)

using $\vec{k} \cdot \vec{R} = kz = kr \cos \theta$. Now in spherical-polar coordinates we have

$$\vec{\mathcal{E}} = \mathcal{E} \left(\sin \theta_{\varepsilon} \cos \varphi_{\varepsilon} \hat{e}_x + \sin \theta_{\varepsilon} \sin \varphi_{\varepsilon} \hat{e}_z + \cos \theta_{\varepsilon} \hat{e}_z \right)$$
(11.170)

$$\vec{r} = r \left(\sin \theta \cos \varphi \hat{e}_x + \sin \theta \sin \varphi \hat{e}_y + \cos \theta \hat{e}_z \right)$$
(11.171)

so that

$$\vec{\mathcal{E}} \cdot \vec{r} = \mathcal{E}r\left(\cos\theta\cos\theta_{\varepsilon} + \sin\theta\sin\theta_{\varepsilon}\cos(\varphi - \varphi_{\varepsilon})\right)$$
(11.172)

We then have

$$\begin{split} \left\langle \vec{k} \middle| \vec{r} \cdot \vec{\mathcal{E}} \middle| 100 \right\rangle \\ &= \frac{2\varepsilon}{a_0^{3/2} L^{3/2}} \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \int dr r^3 e^{-ikr\cos\theta - \frac{r}{a_0}} \left[\cos\theta\cos\theta_{\varepsilon} + \sin\theta\sin\theta_{\varepsilon}\cos(\varphi - \varphi_{\varepsilon}) \right] \end{split}$$

Since

$$\int_{0}^{2\pi} d\varphi \cos \varphi = \int_{0}^{2\pi} d\varphi \sin \varphi = 0$$
(11.173)

the φ - integration wipes out the $\cos(\varphi - \varphi_{\varepsilon})$ term. Letting $x = \cos \theta$ we then have

$$\left\langle \vec{k} \,\middle| \, \vec{r} \cdot \vec{\mathcal{E}} \,\middle| 100 \right\rangle = \frac{4\pi \mathcal{E} \cos\theta_{\varepsilon}}{a_0^{3/2} L^{3/2}} \int_{-1}^{1} \left[\int_{0}^{\infty} dr r^3 e^{-ikrx - \frac{r}{a_0}} \right] x dx \tag{11.174}$$

Now

$$\int_{0}^{\infty} dr r^{3} e^{-ikrx - \frac{r}{a_{0}}} = \int_{0}^{\infty} dr r^{3} e^{-\alpha r} = \frac{3!}{\alpha^{4}} = \frac{6}{\left(ikx + \frac{1}{a_{0}}\right)^{4}}$$
(11.175)

Therefore, we have

$$\left\langle \vec{k} \middle| \vec{r} \cdot \vec{\mathcal{E}} \middle| 100 \right\rangle = \frac{4\pi \mathcal{E} \cos \theta_{\varepsilon}}{a_0^{3/2} L^{3/2}} \int_{-1}^{1} \frac{6x}{\left(ikx + \frac{1}{a_0}\right)^4} dx$$
$$= \frac{4\pi \mathcal{E} \cos \theta_{\varepsilon}}{a_0^{3/2} L^{3/2}} \frac{16ka_0^5}{(1 + k^2 a_0^2)^3}$$
(11.176)

and

$$\left| \left\langle \vec{k} \right| \vec{r} \cdot \vec{\mathcal{E}} \left| 100 \right\rangle \right|^2 = \frac{4096\pi^2 \mathcal{E}^2 \cos^2 \theta_{\varepsilon} a_0^7 k^2}{L^3 (1 + k^2 a_0^2)^6} \tag{11.177}$$

where

$$k^{2} = \frac{2m\omega}{\hbar} - \frac{1}{a_{0}^{2}}$$
(11.178)

Finally, we get

$$\Gamma_{ionization} = \int d\Gamma = \frac{L^3 m k e^2}{16\pi^2 \hbar^3} \int d\Omega_{\vec{k}} \left| \left\langle \vec{k} \right| \vec{r} \cdot \vec{\mathcal{E}} \left| 100 \right\rangle \right|^2 \tag{11.179}$$

where

$$d\Omega_{\vec{k}}$$
 = integration over the angles of \vec{k}
(varies direction of arbitrary z - axis)

However, varying the z-direction is the same as keeping $\vec{\mathcal{E}}$ fixed and integrating over $d\Omega_{\vec{\mathcal{E}}}$. Therefore, we have

$$\Gamma_{ionization} = \frac{L^3 m k e^2}{16\pi^2 \hbar^3} \frac{4096\pi^2 \mathcal{E}^2 a_0^7 k^2}{L^3 (1 + k^2 a_0^2)^6} \int d\Omega_{\vec{\mathcal{E}}} \cos^2 \theta_{\varepsilon}$$
$$= \frac{64\pi m e^2 \mathcal{E}^2 a_0^7}{3\hbar^3} \frac{k^3}{(1 + k^2 a_0^2)^6}$$
(11.180)

Now

$$1 + k^2 a_0^2 = \frac{2m\omega a_0^2}{h} \tag{11.181}$$

and letting

$$\omega_0 = \frac{\hbar}{2ma_0^2} \tag{11.182}$$

we find that

$$1 + k^2 a_0^2 = \frac{\omega}{\omega_0} \text{ and } k = \frac{1}{a_0} \left(\frac{\omega}{\omega_0} - 1\right)^{1/2}$$
 (11.183)

and we get

$$\Gamma_{ionization} = \frac{64\pi e^2 \mathcal{E}^2 a_0^3}{3\hbar} \left(\frac{\omega_0}{\omega}\right)^6 \left(\frac{\omega}{\omega_0} - 1\right)^{3/2}$$
(11.184)

Thus, there exists a threshold energy for this process, i.e., it cannot occur unless the energy of the photon is greater than a minimum amount, which makes physical sense. In particular, we must have $\omega \ge \omega_0$ so that

$$\hbar\omega_0 = |\varepsilon_{100}| = E_{ionization} = \text{ minimum} = \text{threshold}$$
(11.185)

We also get the correct $6^{th}-\mathrm{power}$ term in the answer which agrees with experiment.

11.4 Adiabatic and Sudden Approximations

In standard time-dependent perturbation theory, we assume that the timedependent perturbation is *weak*. An alternative approach, where we assume the time-dependence is *slow*, is called the *adiabatic approximation*.

Suppose that $\hat{H} = \hat{H}(g(t))$, where g(t) tells us the dependence on time. This might correspond to a variation in time of some parameters. We still have

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(g(t)) |\psi(t)\rangle$$
(11.186)

and at any instant of time we have

$$\hat{H}(g(t))|n(g(t))\rangle = E_n(g(t))|n(g(t))\rangle$$
 (11.187)

where n(g(t)) represents the quantum numbers describing the instantaneous state vector.

Let us assume that the instantaneous eigenvectors always form a complete set so that we can write

$$|\psi(t)\rangle = \sum_{n} \alpha_n(t) e^{i\beta_n(t)} |n(g(t))\rangle$$
(11.188)

where we have generalized the phase factor

$$e^{-\frac{i}{\hbar}\varepsilon_n t} \tag{11.189}$$

that appeared in a similar expression in our earlier derivations to include the term

$$\beta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(g(t'))dt'$$
(11.190)

which is called the *dynamical phase*.

Inserting this expression for the state vector $|\psi(t)\rangle$ into the time-dependent

Schrodinger equation we get

$$\begin{split} i\hbar\frac{d}{dt}\sum_{n}\alpha_{n}(t)e^{i\beta_{n}(t)}\left|n(g(t))\right\rangle &= \hat{H}(g(t))\sum_{n}\alpha_{n}(t)e^{i\beta_{n}(t)}\left|n(g(t))\right\rangle \\ i\hbar\sum_{n}\frac{d\alpha_{n}(t)}{dt}e^{i\beta_{n}(t)}\left|n(g(t))\right\rangle &+ i\hbar\sum_{n}\alpha_{n}(t)\frac{de^{i\beta_{n}(t)}}{dt}\left|n(g(t))\right\rangle \\ &+ i\hbar\sum_{n}\alpha_{n}(t)e^{i\beta_{n}(t)}\frac{d}{dt}\left|n(g(t))\right\rangle \\ &= \sum_{n}\alpha_{n}(t)e^{i\beta_{n}(t)}\hat{H}(g(t))\left|n(g(t))\right\rangle &= \sum_{n}\alpha_{n}(t)e^{i\beta_{n}(t)}E_{n}(g(t))\left|n(g(t))\right\rangle \\ i\hbar\sum_{n}\frac{d\alpha_{n}(t)}{dt}e^{i\beta_{n}(t)}\left|n(g(t))\right\rangle &+ i\hbar\sum_{n}\alpha_{n}(t)i\frac{d\beta_{n}(t)}{dt}e^{i\beta_{n}(t)}\left|n(g(t))\right\rangle \\ &+ i\hbar\sum_{n}\alpha_{n}(t)e^{i\beta_{n}(t)}\frac{d}{dt}\left|n(g(t))\right\rangle &= \sum_{n}\alpha_{n}(t)e^{i\beta_{n}(t)}E_{n}(g(t))\left|n(g(t))\right\rangle \end{split}$$

Now

$$\frac{d\beta_n(t)}{dt} = -\frac{1}{\hbar} \frac{d}{dt} \int_0^t E_n(g(t'))dt' = -\frac{1}{\hbar} E_n(g(t))$$
(11.191)

Therefore, we get

$$\sum_{n} \frac{d\alpha_n(t)}{dt} e^{i\beta_n(t)} |n(g(t))\rangle + \sum_{n} \alpha_n(t) e^{i\beta_n(t)} \frac{d}{dt} |n(g(t))\rangle = 0$$
(11.192)

Applying the linear functional

$$\langle m| = \langle m(g(t))| \tag{11.193}$$

from the left we get

$$\sum_{n} \frac{d\alpha_{n}}{dt} e^{i\beta_{n}} \langle m \mid n \rangle + \sum_{n} \alpha_{n} e^{i\beta_{n}} \langle m \mid \frac{d}{dt} \mid n \rangle = 0$$
(11.194)

Using

$$\langle m \mid n \rangle = \delta_{mn} \tag{11.195}$$

we have

$$\frac{d\alpha_m}{dt}e^{i\beta_m} = -\sum_n \alpha_n e^{i\beta_n} \langle m | \frac{d}{dt} | n \rangle$$
(11.196)

$$\frac{d\alpha_m}{dt} = -\sum_n \alpha_n e^{i(\beta_n - \beta_m)} \langle m | \frac{d}{dt} | n \rangle$$
(11.197)

Now taking the time derivative of the eigenvalue equation we have

$$\frac{d\hat{H}}{dt}|n\rangle + \hat{H}\frac{d}{dt}|n\rangle = \frac{dE_n}{dt}|n\rangle + E_n\frac{d}{dt}|n\rangle$$
(11.198)

Again, applying the linear functional $\langle m |$ from the left we get

$$\langle m | \frac{d\hat{H}}{dt} | n \rangle + \langle m | \hat{H} \frac{d}{dt} | n \rangle = \frac{dE_n}{dt} \langle m | n \rangle + E_n \langle m | \frac{d}{dt} | n \rangle$$
(11.199)

For $m \neq n$, using $\langle m | \hat{H} = \langle m | E_m$, we have

$$\langle m | \frac{d\hat{H}}{dt} | n \rangle + E_m \langle m | \frac{d}{dt} | n \rangle = E_n \langle m | \frac{d}{dt} | n \rangle$$
(11.200)

$$\langle m | \frac{d}{dt} | n \rangle = \frac{\langle m | \frac{dH}{dt} | n \rangle}{E_n - E_m} \tag{11.201}$$

Thus, we finally have

$$\frac{d\alpha_m}{dt} = \sum_n \alpha_n e^{i(\beta_n - \beta_m)} \frac{\langle m | \frac{d\hat{H}}{dt} | n \rangle}{E_m - E_n}$$
(11.202)

We choose the *initial* state to be one of the instantaneous eigenvectors

$$|\psi(0)\rangle = |n(g(0))\rangle \tag{11.203}$$

which implies that

$$\alpha_n(0) = 1$$

$$\alpha_m(0) = 0 \quad m \neq n$$

Therefore, for $m \neq n$ at small t we have

$$\frac{d\alpha_m}{dt} \approx e^{i(\beta_n - \beta_m)t} \frac{\langle m | \frac{dH}{dt} | n \rangle}{E_m - E_n}$$
(11.204)

We now assume that

$$\langle m | \frac{dH}{dt} | n \rangle$$
 and $E_m - E_n$ (11.205)

have slow time dependence and that to this order of approximation we can write

$$e^{i(\beta_n - \beta_m)t} = e^{i(E_m - E_n)\frac{t}{\hbar}}$$
(11.206)

which is what we would have if there was no extra time dependence.

We then get

$$\alpha_m(t) \approx -i\hbar \frac{\langle m | \frac{d\hat{H}}{dt} | n \rangle}{(E_m - E_n)^2} \left[e^{i(E_m - E_n)t} - 1 \right]$$
(11.207)

This implies that

$$\alpha_m(t)$$
 remains small for $m \neq n$ (11.208)

The adiabatic theorem assumes that in the case where the system starts in an eigenstate $|n\rangle$ at t = 0, i.e.,

$$\alpha_m(t) = 0 \quad m \neq n \tag{11.209}$$

and that

$$|\psi(t)\rangle = e^{-i\beta_n t} |n(g(t))\rangle \tag{11.210}$$

which says that if the system was in the eigenstate $|n\rangle$ at t = 0, i.e.,

$$\hat{H}(g(0))|n\rangle = \hat{H}_0|n\rangle = \varepsilon_n|n\rangle$$
(11.211)

then at a later time t, it is still in the same eigenstate $|n(g(t))\rangle$ of the new Hamiltonian $\hat{H}(g(t))$, i.e.,

$$\hat{H}(g(t))|n(t)\rangle = E_n(t)|n(t)\rangle \qquad (11.212)$$

This result is *independent* of the size of the perturbation. It depends only on the change in time being *slow*.

This means that if we start with a particle in the ground state of a harmonic oscillator potential

$$V = \frac{1}{2}k(0)x^2 \to \psi_0(k(0), x)$$
(11.213)

and assume that

$$k(0) \to k(T) \tag{11.214}$$

slowly, the particle ends up in the ground state of the harmonic oscillator potential

$$V = \frac{1}{2}k(T)x^2 \to \psi_0(k(T), x)$$
 (11.215)

to within a phase factor.

The opposite result comes from the so-called *sudden approximation*, where the change occurs so fast that no changes of the state vector are possible.

Since the state vector does not change at all, if you are in the ground state and a sudden change in the parameters occurs, then you remain in the ground state for the *old parameters*. This is *not* the ground state with new parameters. It is some *linear combination* of the new states.

Let us look at the adiabatic approximation in another way. We consider a time dependent part of the Hamiltonian of the form

$$\hat{H}(t) = \hat{H}_0 + \hat{H}'$$
, $\hat{H}' = \hat{V}f(t)$ (11.216)

where f(t) has the form shown in Figure 11.5 below.



Figure 11.5: Time Dependence

We assume that the particle starts out in the n^{th} eigenstate of $\hat{H}_0 = \hat{H}(0)$

$$|\psi(0)\rangle = |n\rangle_i \tag{11.217}$$

where the subscripts are

$$i \rightarrow$$
 initial parameters
 $f \rightarrow$ final parameters

The state vectors is assumed to change in time to $|\psi(t)\rangle$.

If \hat{V} is small, we can write, using first order time-independent perturbation theory

$$|m\rangle_{f} = |m\rangle_{i} + \sum_{k \neq m} \frac{V_{km}}{E_{m} - E_{k}} |k\rangle_{i}$$
(11.218)

where

$$V_{km} = {}_i \left\langle k \right| \hat{V} \left| m \right\rangle_i \tag{11.219}$$

On the other hand, first order time-dependent perturbation theory implies that

$$|\psi(t)\rangle = \sum_{n} \alpha_n(t) e^{-\frac{i}{\hbar}E_n t} |n\rangle_i \qquad (11.220)$$

with

$$\alpha_n(t) = 1 - \frac{i}{\hbar} V_{nn} \int_0^t f(t') dt'$$
(11.221)

$$\alpha_m(t) = -\frac{i}{\hbar} V_{mn} \int_0^t f(t') e^{i(E_m - E_n)\frac{t'}{\hbar}} dt' \quad , \quad m \neq n$$
 (11.222)

Now we are assuming that df/dt is small, we integrate by parts to get

$$\begin{aligned} \alpha_m(t) &= -\frac{i}{\hbar} V_{mn} \int_0^t f(t') e^{i(E_m - E_n)\frac{t'}{\hbar}} dt' \\ &= -\frac{V_{mn}}{E_m - E_n} \int_0^t f(t') \frac{d}{dt'} \left[e^{i(E_m - E_n)\frac{t'}{\hbar}} \right] dt' \\ &= -\frac{V_{mn}}{E_m - E_n} \left[f(t') e^{i(E_m - E_n)\frac{t'}{\hbar}} \right]_0^t \\ &+ \frac{V_{mn}}{E_m - E_n} \int_0^t \frac{df(t')}{dt'} e^{i(E_m - E_n)\frac{t'}{\hbar}} dt' \end{aligned}$$
(11.223)

Using f(0) = 0 and neglecting the last term because df/dt is small gives

$$|\psi(T)\rangle = \left[\left(1 - i\frac{V_{nn}}{\hbar}\gamma\right)|n\rangle_i - \sum_{q\neq n} \frac{V_{qn}}{E_q - E_n}|q\rangle_i \right] e^{-\frac{i}{\hbar}E_nT}$$
(11.224)

where

$$\gamma = \int_{0}^{T} f(t)dt \qquad (11.225)$$

Therefore

$$f \langle n | \psi(T) \rangle = \left[i \langle n | + \sum_{k \neq n} \frac{V_{kn}}{E_n - E_k} i \langle k | \right] \left[\left(1 - i \frac{V_{nn}}{\hbar} \gamma \right) | n \rangle_i - \sum_{q \neq n} \frac{V_{qn}}{E_q - E_n} | q \rangle_i \right] e^{-\frac{i}{\hbar} E_n T}$$
$$= \left[1 - i \frac{V_{nn}}{\hbar} \gamma + \sum_{q \neq n} \frac{|V_{qn}|^2}{(E_n - E_q)^2} \right] e^{-\frac{i}{\hbar} E_n T}$$
(11.226)

$$f \langle m \mid \psi(T) \rangle = \left[{}_{i} \langle m \mid + \sum_{k \neq m} \frac{V_{km}}{E_m - E_k} {}_{i} \langle k \mid \right] \left[\left(1 - i \frac{V_{nn}}{\hbar} \gamma \right) | n \rangle_i - \sum_{q \neq n} \frac{V_{qn}}{E_q - E_n} | q \rangle_i \right] e^{-\frac{i}{\hbar} E_n T}$$
$$= \left[-i \gamma \frac{V_{nn} V_{nm}}{\hbar(E_m - E_n)} + \sum_{m \neq k \neq n} \frac{V_{nk} V_{km}}{(E_n - E_k)(E_m - E_k)} \right] e^{-\frac{i}{\hbar} E_n T}$$
(11.227)

Note that all the first order terms cancel in the last expression. If we only keep terms to first order (which is consistent with the derivation) we then have

$$_{f}\left\langle k\left|\psi(T)\right\rangle =\begin{cases} \left[1-i\frac{V_{nn}}{\hbar}\gamma\right] & k=n\\ 0 & k\neq n \end{cases}$$
(11.228)

which implies that

 $\begin{aligned} |_{f} \langle n | \psi(T) \rangle|^{2} &= 1 + \frac{|V_{nn}|^{2} \gamma^{2}}{\hbar^{2}} \to 1 \text{ to first order} \\ |_{f} \langle m | \psi(T) \rangle|^{2} &= 0 \text{ to first order } m \neq n \end{aligned}$

which is the *adiabatic approximation*.

Therefore, the adiabatic approximation says:

if the Hamiltonian $\hat{H}(t)$ changes slowly in time, then there will be no transitions from the eigenstate $|n\rangle_i$ of $\hat{H}(0)$ to a *different* eigenstate $|m\rangle_f$ of $\hat{H}(t)$

In time-dependent perturbation theory, we assume the perturbation is turned on and off and thus $\hat{H}(0) = \hat{H}(T)$, i.e., we have the *same* unperturbed Hamiltonian at the end.

The transitions in that case are from one eigenvector of the unperturbed Hamiltonian to another eigenvector of the same unperturbed Hamiltonian.

This implies a first-order transition amplitude and hence a second-order transition probability.

In the adiabatic approximation, however, we have a second-order transition amplitude $(m \neq n)$ and hence a fourth-order transition probability. That is why we can assume that the transition probability for $m \neq n$ is equal to zero.

The first derivation gives the adiabatic approximation for any size perturbation. In the second derivation, however, we not only assumed a slow change in time, but also assumes a small perturbation so that we could use first order perturbation theory.

What happens in the second derivation if the perturbation is not small?

The way to handle this is to divide the time interval (0,T) into N subintervals such that the perturbation ΔV is small within any subinterval. In fact, it is of O(V/N). Thus, if N is large, ΔV is small.

We then apply our arguments to each subinterval. If the transition amplitude is first-order in the perturbation, then the total transition amplitude behaves like

$$N\left(\frac{V}{N}\right) \to V$$
 (11.229)

with each of the N steps giving a contribution proportional to ΔV . This says that the net result is of order V, and thus, if V is large, the transition amplitude will be large.

However, the transition amplitude is second-order and thus the total transition

amplitude behaves like

$$N\left(\frac{V}{N}\right)^2 \to \frac{V^2}{N} \to 0 \text{as} N \to \infty$$
 (11.230)

Therefore, the transition amplitude $(m \neq n)$ is zero *independent of the size* of V.

An Example

Let us consider a 1–dimensional square well where

$$V(x) = \begin{cases} 0 & |x| \le \frac{a}{2} \\ \infty & |x| > \frac{a}{2} \end{cases}$$
(11.231)

The eigenfunctions and energies are

$$\psi_n(x) = \begin{cases} \cos \frac{n\pi x}{2a} & n = 1, 3, 5, \dots \\ \sin \frac{n\pi x}{2a} & n = 2, 4, 6, \dots \end{cases}$$
(11.232)

for $|x| \leq \frac{a}{2}$ and zero otherwise and

$$E_n = \frac{\pi^2 \hbar^2 n^2}{8ma^2} \quad n = 1, 2, 3, \dots ...$$
(11.233)

Suppose that we change the size of the well and ask what happens to the ground state in the sudden and adiabatic approximations.

Sudden

$$\psi_1(x) = \cos \frac{\pi x}{2a} \text{ before} \tag{11.234}$$

leads to

$$\psi(x) = \cos \frac{\pi x}{2a}$$
 after (no change in the wave function) (11.235)

However, after the change we have new eigenfunctions and energies

$$\psi_n'(x) = \begin{cases} \cos \frac{n\pi x}{4\bar{a}} & n = 1, 3, 5, \dots \\ \sin \frac{n\pi x}{4\bar{a}} & n = 2, 4, 6, \dots \end{cases}$$
(11.236)

for $|x| \leq \frac{a}{2}$ and zero otherwise and

$$E'_{n} = \frac{\pi^{2} \hbar^{2} n^{2}}{8m\bar{a}^{2}} \quad n = 1, 2, 3, \dots \dots$$
(11.237)

The state of the system is still an eigenstate of the old well and, thus, is *not* an eigenstate of the new well. In fact, we have

$$\psi(x) = \cos\frac{\pi x}{2a} = \sum_{n} b_n \psi'_n(x)$$
 (11.238)

Adiabatic

$$\psi_1(x) = \cos \frac{\pi x}{2a}$$
 before (ground state of old well) (11.239)

$$\psi'_1(x) = \cos \frac{\pi x}{4a}$$
 after (ground state of new well) (11.240)

The state of the system is an eigenstate of the new well and, thus, is *not* an eigenstate of the old well any longer. In fact, we have

$$\psi'_{n}(x) = \cos \frac{\pi x}{4a} = \sum_{n} b_{n} \psi_{n}(x)$$
 (11.241)

It is a superposition of the old energy eigenstates.

11.5 Problems

11.5.1 Square Well Perturbed by an Electric Field

At time t = 0, an electron is known to be in the n = 1 eigenstate of a 1-dimensional infinite square well potential

$$V(x) = \begin{cases} \infty & \text{for } |x| > a/2\\ 0 & \text{for } |x| < a/2 \end{cases}$$

At time t = 0, a uniform electric field of magnitude \mathcal{E} is applied in the direction of increasing x. This electric field is left on for a short time τ and then removed. Use time-dependent perturbation theory to calculate the probability that the electron will be in the n = 2, 3 eigenstates at some time $t > \tau$.

11.5.2 3-Dimensional Oscillator in an electric field

A particle of mass M, charge e, and spin zero moves in an attractive potential

$$V(x, y, z) = k \left(x^2 + y^2 + z^2 \right)$$
(11.242)

- (a) Find the three lowest energy levels E_0 , E_1 , E_2 and their associated degeneracy.
- (b) Suppose a small perturbing potential $Ax \cos \bar{\omega}t$ causes transitions among the various states in (a). Using a convenient basis for degenerate states, specify in detail the allowed transitions neglecting effects proportional to A^2 or higher.
- (c) In (b) suppose the particle is in the ground state at time t = 0. Find the probability that the energy is E_1 at time t.

11.5.3 Hydrogen in decaying potential

A hydrogen atom (assume spinless electron and proton) in its ground state is placed between parallel plates and subjected to a uniform weak electric field

$$\vec{\mathcal{E}} = \begin{cases} 0 & \text{for } t < 0 \\ \vec{\mathcal{E}}_0 e^{-\alpha t} & \text{for } t > 0 \end{cases}$$

Find the 1^{st} order probability for the atom to be in any of the n = 2 states after a long time.

11.5.4 2 spins in a time-dependent potential

Consider a composite system made up of two spin = 1/2 objects. For t < 0, the Hamiltonian does not depend on spin and can be taken to be zero by suitably adjusting the energy scale. For t > 0, the Hamiltonian is given by

$$\hat{H} = \left(\frac{4\Delta}{\hbar^2}\right)\vec{S}_1 \cdot \vec{S}_2$$

Suppose the system is in the state $|+-\rangle$ for $t \leq 0$. Find, as a function of time, the probability for being found in each of the following states $|++\rangle$, $|-+\rangle$ and $|--\rangle$.

- (a) by solving the problem exactly.
- (b) by solving the problem assuming the validity of 1^{st} -order time-dependent perturbation theory with \hat{H} as a perturbation switched on at t = 0. Under what conditions does this calculation give the correct results?

11.5.5 A Variational Calculation of the Deuteron Ground State Energy

Use the empirical potential energy function

$$V(r) = -Ae^{-r/a}$$

where A = 32.7 MeV, $a = 2.18 \times 10^{-13} cm$, to obtain a variational approximation to the energy of the ground state energy of the deuteron ($\ell = 0$).

Try a simple variational function of the form

$$\phi(r) = e^{-\alpha r/2a}$$

where α is the variational parameter to be determined. Calculate the energy in terms of α and minimize it. Give your results for α and E in MeV. The experimental value of E is -2.23 MeV (your answer should be VERY close! Is your answer above this? [HINT: do not forget about the *reduced mass* in this problem]

11.5.6 Sudden Change - Don't Sneeze

An experimenter has carefully prepared a particle of mass m in the first excited state of a one dimensional harmonic oscillator, when he sneezes and knocks the center of the potential well a small distance a to one side. It takes him a time T to blow his nose, and when he has done so, he immediately puts the center back where it was. Find, to lowest order in a, the probabilities P_0 and P_2 that the oscillator will now be in its ground state and its second excited state.

11.5.7 Another Sudden Change - Cutting the spring

A particle is allowed to move in one dimension. It is initially coupled to two identical harmonic springs, each with spring constant K. The springs are symmetrically fixed to the points $\pm a$ so that when the particle is at x = 0 the classical force on it is zero.

- (a) What are the energy eigenvalues of the particle when it is connected to both springs?
- (b) What is the wave function in the ground state?
- (c) One spring is suddenly cut, leaving the particle bound to only the other one. If the particle is in the ground state before the spring is cut, what is the probability that it is still in the ground state after the spring is cut?

11.5.8 Another perturbed oscillator

Consider a particle bound in a simple harmonic oscillator potential. Initially (t < 0), it is in the ground state. At t = 0 a perturbation of the form

$$H'(x,t) = Ax^2 e^{-t/\tau}$$

is switched on. Using time-dependent perturbation theory, calculate the probability that, after a sufficiently long time $(t \gg \tau)$, the system will have made a transition to a given excited state. Consider all final states.

11.5.9 Nuclear Decay

Nuclei sometimes decay from excited states to the ground state by internal conversion, a process in which an atomic electron is emitted instead of a photon. Let the initial and final nuclear states have wave functions $\varphi_i(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z)$ and $\varphi_f(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z)$, respectively, where \vec{r}_i describes the protons. The perturbation giving rise to the transition is the proton-electron interaction,

$$W = -\sum_{j=1}^{Z} \frac{e^2}{|\vec{r} - \vec{r}_j|}$$

where \vec{r} is the electron coordinate.

- (a) Write down the matrix element for the process in lowest-order perturbation theory, assuming that the electron is initially in a state characterized by the quantum numbers $(n\ell m)$, and that its energy, after it is emitted, is large enough so that its final state may be described by a plane wave, Neglect spin.
- (b) Write down an expression for the internal conversion rate.
- (c) For light nuclei, the nuclear radius is much smaller than the Bohr radius for a give Z, and we can use the expansion

$$\frac{1}{|\vec{r}-\vec{r}_j|}\approx \frac{1}{r}+\frac{\vec{r}\cdot\vec{r}_j}{r^3}$$

Use this expression to express the transition rate in terms of the dipole matrix element

$$\vec{d} = \left\langle \varphi_f \right| \sum_{j=1}^{Z} \vec{r}_j \left| \varphi_i \right\rangle$$

11.5.10 Time Evolution Operator

A one-dimensional anharmonic oscillator is given by the Hamiltonian

$$H = \hbar\omega \left(a^{\dagger}a + 1/2 \right) + \lambda a^{\dagger}aa$$

where λ is a constant. First compute a^+ and a in the interaction picture and then calculate the time evolution operator $U(t, t_0)$ to lowest order in the perturbation.

11.5.11 Two-Level System

Consider a two-level system $|\psi_a\rangle$, $|\psi_b\rangle$ with energies E_a , E_b perturbed by a jolt $H'(t) = \hat{U}\delta(t)$ where the operator \hat{U} has only off-diagonal matrix elements (call them U). If the system is initially in the state a, find the probability $P_{a\to b}$ that a transition occurs. Use only the lowest order of perturbation theory that gives a nonzero result.

11.5.12 Instantaneous Force

Consider a simple harmonic oscillator in its ground state. An instantaneous force imparts momentum p_0 to the system. What is the probability that the system will stay in its ground state?

11.5.13 Hydrogen beam between parallel plates

A beam of excited hydrogen atoms in the 2s state passes between the plates of a capacitor in which a uniform electric field exists over a distance L. The hydrogen atoms have a velocity v along the x-axis and the electric field $\vec{\mathcal{E}}$ is directed along the z-axis as shown in the figure.



Figure 11.6: Hydrogen beam between parallel plates

All of the n = 2 states of hydrogen are degenerate in the absence of the field $\vec{\mathcal{E}}$, but certain of them mix (Stark effect) when the field is present.

- (a) Which of the n = 2 states are connected (mixed) in first order via the electric field perturbation?
- (b) Find the linear combination of the n = 2 states which removes the degeneracy as much as possible.
- (c) For a system which starts out in the 2s state at t = 0, express the wave function at time $t \leq L/v$. No perturbation theory needed.
- (d) Find the probability that the emergent beam contains hydrogen in the various n = 2 states.

11.5.14 Particle in a Delta Function and an Electric Field

A particle of charge q moving in one dimension is initially bound to a delta function potential at the origin. From time t = 0 to $t = \tau$ it is exposed to a constant electric field \mathcal{E}_0 in the *x*-direction as shown in the figure below:



Figure 11.7: Electric Field

The object of this problem is to find the probability that for $t > \tau$ the particle will be found in an unbound state with energy between E_k and $E_k + dE_k$.

- (a) Find the normalized bound-state energy eigenfunction corresponding to the delta function potential $V(x) = -A\delta(x)$.
- (b) Assume that the unbound states may be approximated by free particle states with periodic boundary conditions in a box of length L. Find the normalized wave function of wave vector k, $\psi_k(x)$, the density of states as

a function of k, D(k) and the density of states as a function of free-particle energy E_k , $D(E_k)$.

- (c) Assume that the electric field may be treated as a perturbation. Write down the perturbation term in the Hamiltonian, \hat{H}_1 , and find the matrix element of \hat{H}_1 between the initial and the final state $\langle 0|\hat{H}_1|k \rangle$.
- (d) The probability of a transition between an initially occupied state $|I\rangle$ and a final state $|F\rangle$ due to a weak perturbation $\hat{H}_1(t)$ is given by

$$P_{I \to F}(t) = \frac{1}{\hbar^2} \left| \int_{-\infty}^t \langle F | \hat{H}_1(t') | I \rangle e^{i\omega_{FI}t'} dt' \right|^2$$

where $\omega_{FI} = (E_F - E_I)/\hbar$. Find an expression for the probability $P(E_k)dE_k$ that the particle will be in an unbound state with energy between E_k and $E_k + dE_k$ for $t > \tau$.

11.5.15 Nasty time-dependent potential [complex integration needed]

A one-dimensional simple harmonic oscillator of frequency ω is acted upon by a time-dependent, but spatially uniform force (not potential!)

$$F(t) = \frac{(F_0 \tau/m)}{\tau^2 + t^2} , \quad -\infty < t < \infty$$

At $t = -\infty$, the oscillator is known to be in the ground state. Using timedependent perturbation theory to 1^{st} -order, calculate the probability that the oscillator is found in the 1^{st} excited state at $t = +\infty$.

Challenge: F(t) is so normalized that the impulse

$$\int F(t)dt$$

imparted to the oscillator is always the same, that is, independent of τ ; yet for $\tau \gg 1/\omega$, the probability for excitation is essentially negligible. Is this reasonable?

11.5.16 Natural Lifetime of Hydrogen

Though in the absence of any perturbation, an atom in an excited state will stay there forever(it is a stationary state), in reality, it will *spontaneously decay* to the ground state. Fundamentally, this occurs because the atom is always perturbed by vacuum fluctuations in the electromagnetic field. The spontaneous emission rate on a dipole allowed transition from the initial excited state $|\psi_e\rangle$ to all allowed ground states $|\psi_g\rangle$ is,

$$\Gamma = \frac{4}{3\hbar}k^3 \sum_{g} \left| \langle \psi_g | \hat{\vec{d}} | \psi_e \rangle \right|^2$$

where $k = \omega_{eg}/c = (E_e - E_g)/\hbar c$ is the emitted photon's wave number.

Consider now hydrogen including fine structure. For a given sublevel, the spontaneous emission rate is

$$\Gamma_{(nLJM_J)\to(n'L'J')} = \frac{4}{3\hbar}k^3 \sum_{M'_J} \left| \langle n'L'J'M'_J | \vec{d} | nLJM_J \rangle \right|^2$$

- (a) Show that the spontaneous emission rate is independent of the initial M_J . Explain this result physically.
- (b) Calculate the lifetime $(\tau = 1/\Gamma)$ of the $2P_{1/2}$ state in seconds.

11.5.17 Oscillator in electric field

Consider a simple harmonic oscillator in one dimension with the usual Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2$$

Assume that the system is in its ground state at t = 0. At t = 0 an electric field $\vec{\mathcal{E}} = \mathcal{E}\hat{x}$ is switched on, adding a term to the Hamiltonian of the form

$$H' = e\mathcal{E}\hat{x}$$

- (a) What is the new ground state energy?
- (b) Assuming that the field is switched on in a time much faster than 1/ω, what is the probability that the particle stays in the unperturbed ground state?

11.5.18 Spin Dependent Transitions

Consider a spin= 1/2 particle of mass m moving in three kinetic dimensions, subject to the spin dependent potential

$$\hat{V}_{1} = \frac{1}{2}k\left|-\right\rangle\left\langle-\right| \otimes \left|\vec{r}\right|^{2}$$

where k is a real positive constant, \vec{r} is the three-dimensional position operator, and $\{|-\rangle, |+\rangle\}$ span the spin part of the Hilbert space. Let the initial state of the particle be prepared as

$$|\Psi_0\rangle = |-\rangle \otimes |0\rangle$$

where $|0\rangle$ corresponds to the ground state of the harmonic (motional) potential.

(a) Suppose that a perturbation

$$\hat{W} = \hbar \Omega \left(\left| - \right\rangle \left\langle + \right| + \left| + \right\rangle \left\langle - \right| \right) \otimes \hat{I}^{CM}$$

where \hat{I}^{CM} denotes the identity operator on the motional Hilbert space, is switched on at time t = 0.

Using Fermi's Golden Rule compute the rate of transitions out of $|\Psi_0\rangle$.

- (b) Describe qualitatively the evolution induced by \hat{W} , in the limits $\Omega \gg \sqrt{k/m}$ and $\Omega \ll \sqrt{k/m}$. HINT: Make sure you understand part(c).
- (c) Consider a different spin-dependent potential

$$\hat{V}_2 = |+\rangle \langle +| \otimes \Sigma_+(\vec{x}) + |-\rangle \langle -| \otimes \Sigma_-(\vec{x}) \rangle$$

where $\Sigma_{\pm}(\vec{x})$ denote the motional potentials

$$\Sigma_{+}(\vec{x}) = \begin{cases} +\infty & |x| < a \\ 0 & |x| \ge a \end{cases}$$
$$\Sigma_{-}(\vec{x}) = \begin{cases} 0 & |x| < a \\ +\infty & |x| \ge a \end{cases}$$

and a is a positive real constant. Let the initial state of the system be prepared as

$$|\Psi_0\rangle = |-\rangle \otimes |0'\rangle$$

where $|0'\rangle$ corresponds to the ground state of $\Sigma_{-}(\vec{x})$. Explain why Fermi's Golden Rule predicts a vanishing transition rate for the perturbation \hat{W} specified in part (a) above.

11.5.19 The Driven Harmonic Oscillator

At t=0 a 1–dimensional harmonic oscillator with natural frequency ω is driven by the perturbation

$$H_1(t) = -Fxe^{-i\Omega t}$$

The oscillator is initially in its ground state at t = 0.

- (a) Using the lowest order perturbation theory to get a nonzero result, find the probability that the oscillator will be in the 2nd excited state n = 2 at time t > 0. Assume $\omega \neq \Omega$.
- (b) Now begin again and do the simpler case, $\omega = \Omega$. Again, find the probability that the oscillator will be in the 2nd excited state n = 2 at time t > 0
- (c) Expand the result of part (a) for small times t, compare with the results of part (b), and interpret what you find.

In discussing the results see if you detect any parallels with the driven classical oscillator.

11.5.20 A Novel One-Dimensional Well

Using tremendous skill, physicists in a molecular beam epitaxy lab, use a graded semiconductor growth technique to make a GaAs(Gallium Arsenide) wafer containing a single 1-dimensional (Al,Ga)As quantum well in which an electron is confined by the potential $V = kx^2/2$.

- (a) What is the Hamiltonian for an electron in this quantum well? Show that $\psi_0(x) = N_0 e^{-\alpha x^2/2}$ is a solution of the time-independent Schrödinger equation with this Hamiltonian and find the corresponding eigenvalue. Assume here that $\alpha = m\omega/\hbar$, $\omega = \sqrt{k/m}$ and m is the mass of the electron. Also assume that the mass of the electron in the quantum well is the same as the free electron mass (not always true in solids).
- (b) Let us define the raising and lowering operators \hat{a} and \hat{a}^{\dagger} as

$$\hat{a}^+ = \frac{1}{\sqrt{2}} \left(\frac{d}{dy} - y \right) \quad , \quad \hat{a} = \frac{1}{\sqrt{2}} \left(\frac{d}{dy} + y \right)$$

where $y = \sqrt{m\omega/\hbar x}$. Find the wavefunction which results from operating on ψ_0 with \hat{a}^+ (call it $\psi_1(x)$). What is the eigenvalue of ψ_1 in this quantum well? You can just state the eigenvalue based on your knowledge - there is no need to derive it.

- (c) Write down the Fermi's Golden Rule expression for the rate of a transition (induced by an oscillating perturbation from electromagnetic radiation) occuring between the lowest energy eigenstate and the first excited state. State the assumptions that go into the derivation of the expression.
- (d) Given that $k = 3.0 kg/s^2$, what photon wavelength is required to excite the electron from state ψ_0 to state ψ_1 ? Use symmetry arguments to decide whether this is an allowed transition (explain your reasoning); you might want to sketch $\psi_0(x)$ and $\psi_1(x)$ to help your explanation.
- (e) Given that

$$\hat{a}|\nu\rangle = \sqrt{\nu}|\nu-1\rangle$$
 , $\hat{a}^{+}|\nu\rangle = -\sqrt{\nu+1}|\nu+1\rangle$

evaluate the transition matrix element $\langle 0|x|1 \rangle$. (HINT: rewrite x in terms of \hat{a} and \hat{a}^+). Use your result to simplify your expression for the transition rate.

11.5.21 The Sudden Approximation

Suppose we specify a three-dimensional Hilbert space \mathcal{H}_A and a time-dependent Hamiltonian operator

$$H(t) = \alpha \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} + \beta(t) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -2 \end{pmatrix}$$

where α and $\beta(t)$ are real-valued parameters (with units of energy). Let $\beta(t)$ be given by a step function

$$\beta(t) = \begin{cases} \alpha & t \le 0\\ 0 & t > 0 \end{cases}$$

The Schrodinger equation can clearly be solved by standard methods in the intervals $t = [-\infty, 0]$ and $t = (0, +\infty]$, within each of which H remains constant. We can use the so-called *sudden approximation* to deal with the discontinuity in H at t = 0, which simply amounts to assuming that

$$|\Psi(0_+)\rangle = |\Psi(0_-)\rangle$$

Suppose the system is initially prepared in the ground state of the Hamiltonian at t = -1. Use the Schrödinger equation and the sudden approximation to compute the subsequent evolution of $|\Psi(t)\rangle$ and determine the function

$$f(t) = \langle |\Psi(0)\rangle | |\Psi(t)\rangle\rangle \quad , \quad t \ge 0$$

Show that $|f(t)|^2$ is periodic. What is the frequency? How is it related to the Hamiltonian?

11.5.22 The Rabi Formula

Suppose the total Hamiltonian for a spin-1/2 particle is

$$H = -\gamma \left[B_0 S_z + b_1 \left(\cos \left(\omega t \right) S_x + \sin \left(\omega t \right) S_y \right) \right]$$

which includes a static field B_0 in the z direction plus a rotating field in the x - y plane. Let the state of the particle be written

$$|\Psi(t)\rangle = a(t)|+_z\rangle + b(t)|-_z\rangle$$

with normalization $|a|^2 + |b|^2 = 1$ and initial conditions

$$a(0) = 0$$
 , $b(0) = 1$

Show that

$$|a(t)|^{2} = \frac{(\gamma b_{1})^{2}}{\Delta^{2} + (\gamma b_{1})^{2}} \sin^{2} \left(\frac{t}{2}\sqrt{\Delta^{2} + (\gamma b_{1})^{2}}\right)$$

where $\Delta = -\gamma B_0 - \omega$. This expression is known as the *Rabi Formula*.

11.5.23 Rabi Frequencies in Cavity QED

Consider a two-level atom whose pure states can be represented by vectors in a two-dimensional Hilbert space \mathcal{H}_A . Let $|g\rangle$ and $|e\rangle$ be a pair of orthonormal basis states of \mathcal{H}_A representing the ground and excited states of the atom, respectively. Consider also a microwave cavity whose lowest energy pure states can be

described by vectors in a three-dimensional Hilbert space \mathcal{H}_C . Let $\{|0\rangle, |1\rangle, |2\rangle\}$ be orthonormal basis states representing zero, one and two microwave photons in the cavity.

The experiment is performed by sending a stream of atoms through the microwave cavity. The atoms pass through the cavity one-by-one. Each atom spends a total time t inside the cavity (which can be varied by adjusting the velocities of the atoms). Immediately upon exiting the cavity each atom hits a detector that measures the atomic projection operator $P_e = |e\rangle \langle e|$.

Just before each atom enters the cavity, we can assume that the joint state of that atom and the microwave cavity is given by the factorizable pure state

$$|\Psi(0)\rangle = |g\rangle \otimes (c_0|0\rangle + c_1|1\rangle + c_2|2\rangle)$$

where $|c_0|^2 + |c_1|^2 + |c_2|^2 = 1$

(a) Suppose the Hamiltonian for the joint atom-cavity system vanishes when the atom is not inside the cavity and when the atom is inside the cavity the Hamiltonian is given by

$$H_{AC} = \hbar\nu |e\rangle \langle g| \otimes \left(|0\rangle \langle 1| + \sqrt{2} |1\rangle \langle 2|\right) + \hbar\nu |g\rangle \langle e| \otimes \left(|1\rangle \langle 0| + \sqrt{2} |2\rangle \langle 1|\right)$$

Show that while the atom is inside the cavity, the following joint states are eigenstates of H_{AC} and determine the eigenvalues:

$$|E_{0}\rangle = |g\rangle \otimes |0\rangle$$

$$|E_{1+}\rangle = \frac{1}{\sqrt{2}} (|g\rangle \otimes |1\rangle + |e\rangle \otimes |0\rangle)$$

$$|E_{1-}\rangle = \frac{1}{\sqrt{2}} (|g\rangle \otimes |1\rangle - |e\rangle \otimes |0\rangle)$$

$$|E_{2+}\rangle = \frac{1}{\sqrt{2}} (|g\rangle \otimes |2\rangle + |e\rangle \otimes |1\rangle)$$

$$|E_{2-}\rangle = \frac{1}{\sqrt{2}} (|g\rangle \otimes |2\rangle - |e\rangle \otimes |1\rangle)$$

Then rewrite $|\Psi(0)\rangle$ as a superposition of energy eigenstates.

(b) Use part (a) to compute the expectation value

$$\langle P_e \rangle = \langle \Psi(t) | P_e \otimes I^C | \Psi(t) \rangle$$

as a function of atomic transit time t. You should find your answer is of the form

$$\langle P_e \rangle = \sum_n P(n) \sin^2 \left[\Omega_n t \right]$$

where P(n) is the probability of having *n* photons in the cavity and Ω_n is the *n*-photon Rabi frequency.

Chapter 12

Identical Particles

12.1 Theoretical ideas

We now apply these quantum mechanical methods we have developed to multielectron atoms.

We will create a model to handle these atoms that follows from the one-electron case we just considered. These systems are very complex and all the results that we derive will be approximations.

If we consider an atom or system of N particles, the wave function

$$\psi(1, 2, 3, 4, \dots, N, t) = \psi(\vec{r}_1 s_1, \vec{r}_2 s_2, \vec{r}_3 s_3, \vec{r}_4 s_4, \dots, \vec{r}_N s_N, t)$$

= $\langle 1, 2, 3, 4, \dots, N, t | \psi \rangle$ (12.1)
where $\vec{r}_j s_j$ = (radius vector, spin) of the j^{th} particle

describing the system will be a function of 3N spatial coordinates, time and all of the particle spin variables. The 3N spatial coordinates form a multidimensional configuration space.

The Hamiltonian of the system is given by

$$\hat{H} = \hat{T} + \hat{V} \tag{12.2}$$

where

$$\hat{T} = \sum_{j=1}^{N} \hat{T}_{j} = -\sum_{j=1}^{N} \left(\frac{\hbar^{2}}{2m_{j}} \nabla_{j}^{2} \right) \text{ and } \hat{V} = \hat{V}(\vec{r}_{1}, \vec{r}_{2}, \dots, \vec{r}_{N}, t)$$
(12.3)

The time-dependent Schrodinger equation is

$$\hat{H}\psi(1,2,3,4,...,N,t) = i\hbar \frac{\partial}{\partial t}\psi(1,2,3,4,...,N,t)$$
(12.4)

The probability density is defined as

$$\rho(1,2,3,4,\ldots,N,t) = \psi^*(1,2,3,4,\ldots,N,t)\psi(1,2,3,4,\ldots,N,t)$$
(12.5)

so that

$$\rho(1,2,3,4,\ldots,N,t)d^3\vec{r}_1d^3\vec{r}_2\ldots d^3\vec{r}_N = \text{ probability of finding}$$

particle 1 at \vec{r}_1 in $d^3\vec{r}_1$, and particle 2 at \vec{r}_2 in $d^3\vec{r}_2$,
...., and particle N at \vec{r}_N in $d^3\vec{r}_N$ all at time time t

We assume that the N-particle wave function is normalized.

The energy eigenstates or stationary states are solutions of

$$\hat{H}\psi_E(1,2,3,4,...,N) = E\psi_E(1,2,3,4,...,N)$$
 (12.6)

which implies the time dependence

$$\psi(1,2,3,4,\ldots,N,t) = \psi_E(1,2,3,4,\ldots,N)e^{-i\frac{D}{h}t}$$
(12.7)

where E is the energy of the system.

When we consider an N-electron atom, the system really has N + 1 particles (we must include the nucleus). However, the nucleus is so much more massive than the electrons that we can make the approximation that it has infinite mass and is fixed.

We put the nucleus of charge Ze at the origin and define

 \vec{r}_j = position vector of the j^{th} electron $r_{jk} = |\vec{r}_j - \vec{r}_k|$ = separation between the j^{th} and k^{th} electrons

The potential energy is

$$V(1, 2, 3,, N) = -\sum_{j=1}^{N} \frac{Ze^2}{r_j} + \sum_{j=1}^{N} \sum_{i>j}^{N} \frac{e^2}{r_{ij}}$$

$$= \text{Coulomb energy between nucleus and electrons}$$

$$+ \text{Coulomb energy between electrons}$$
(12.8)

We will assume no spin-dependence or time dependence in the potential energy.

All electrons in the atom are considered to be *identical* or *indistinguishable*. This means that there are no interactions that can, in any way, distinguish them from each other.

Alternatively, we can say that, if we interchange the coordinates and spins of two particles, then it is not possible to determine via any physical measurement that any change was made in the system.

This says that all measurable quantities or the operators representing them must

remain unchanged by the interchange of indistinguishable particles.

In particular, the Hamiltonian must remain unchanged, i.e., we must have

$$\hat{H}(1,2,3,4,...,j,k,...,N) = \hat{H}(1,2,3,4,...,k,j,...,N)$$
(12.9)

This property of \hat{H} is called *exchange symmetry*. Operators that have this property are *symmetric* functions of their indices $1, 2, 3, 4, \dots, N$ and they are called *symmetric* operators.

Now, every symmetry of a physical system must be represented by an operator that commutes with \hat{H} . In this case, we introduce the *particle interchange* or *permutation operator* \hat{P}_{ij} such that

$$\hat{P}_{ij}\psi(1,2,3,...,i,j,...,N) = \langle 1,2,3,...,i,j,...,N | \hat{P}_{ij} | \psi \rangle$$

= $\langle 1,2,3,...,j,i,...,N | \psi \rangle = \psi(1,2,3,...,j,i,...,N)$

In words, we say

 $\hat{P}_{ij}\psi(1,2,3,...,i,j,...,N)$ gives the amplitude for finding the j^{th} particle at \vec{r}_i with spin s_i and i^{th} particle at \vec{r}_j with spin s_j

. . .

Now, the transformed Hamiltonian operator is given by

.

$$\hat{H}' = \hat{P}_{ij}\hat{H}\hat{P}_{ij}^{-1} = \hat{H} \text{ (by assumption)}$$
(12.10)

This implies that

$$\hat{P}_{ij}\hat{H} = \hat{H}\hat{P}_{ij} \rightarrow \left[\hat{H}, \hat{P}_{ij}\right] = 0 \tag{12.11}$$

as we expected. The same result holds for all symmetric operators.

Now, suppose that the state vector $|\psi\rangle$ is an eigenvector of the symmetric, N-particle \hat{H} with energy E. We then have

$$H\left|\psi\right\rangle = E\left|\psi\right\rangle \tag{12.12}$$

$$\hat{H}\hat{P}_{ij}|\psi\rangle = \hat{P}_{ij}\hat{H}|\psi\rangle = E\hat{P}_{ij}|\psi\rangle \qquad (12.13)$$

which says that

$$P_{ij} |\psi\rangle$$
 is also an eigenvector of H with the same energy (12.14)

This holds for any pair (i, j). So \hat{H} and \hat{P}_{ij} share a common eigenbasis as expected. This phenomenon is called *exchange degeneracy*.

For simplicity, we assume that N = 2. We then have

$$\hat{H}(1,2) \text{ and } \psi(1,2)$$
 (12.15)

and

$$\left[\hat{H}, \hat{P}_{12}\right] = 0 \tag{12.16}$$

What are the simultaneous eigenfunctions? We have

$$\hat{P}_{12}\psi(1,2) = \psi(2,1)$$
$$\hat{P}_{12}^2\psi(1,2) = \hat{P}_{12}\psi(2,1) = \psi(1,2)$$

which says that

$$\hat{P}_{12}^2 = \hat{I} \tag{12.17}$$

and that \hat{P}_{12} has eigenvalues ± 1 . Now if

$$\hat{H}\psi(1,2) = E\psi(1,2)$$
 (12.18)

then

$$\hat{H}\psi(2,1) = E\psi(2,1)$$
 (12.19)

and these two state functions are degenerate. Then, we can write

$$\psi_S(1,2) = \psi(1,2) + \psi(2,1) \rightarrow \text{symmetric wave function}$$

 $\psi_A(1,2) = \psi(1,2) - \psi(2,1) \rightarrow \text{antisymmetric wave function}$

which are the simultaneous eigenfunctions with

$$\hat{H}\psi_S = E\psi_S \qquad \hat{H}\psi_A = E\psi_A \tag{12.20}$$

$$\hat{P}_{12}\psi_S = +\psi_S \qquad \hat{P}_{12}\psi_A = -\psi_A$$
 (12.21)

It is an *experimental fact* that the behavior of wave functions under pairwise particle interchange depends only on the kind of particles involved, in particular on their *spin*.

All known particles divide themselves in to two classes:

- 1. Bosons \rightarrow particles with integer spin, $s = 0, 1, 2, 3, 4, \dots$
- 2. Fermions \rightarrow particles with half-integer spin, $s = 1/2, 3/2, 5/2, \dots$

and

- 1. Fermions have antisymmetric wave functions under particle interchange
- 2. Bosons have symmetric wave functions under particle interchange

This relationship between spin and wave function symmetry cannot be proved in non-relativistic quantum mechanics. It can, however, be proved if we add relativity and construct the relativistic waves equations for bosons and fermions.

As we shall see, this symmetry/antisymmetry connection of spin and wave functions will generalize to more complex systems with more particles. Before proceeding to study real atoms with N electrons, let us see what we can learn from a one-dimensional systems containing either two identical bosons or two identical fermions.

The general Hamiltonian for a one-dimensional two-particle system is

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{U}(x_1 - x_2)$$
(12.22)

$$\hat{H}_{1} = -\frac{\hbar^{2}}{2m} \frac{\partial^{2}}{\partial x_{1}^{2}} + \hat{V}(x_{1})$$
(12.23)

$$\hat{H}_{2} = -\frac{\hbar^{2}}{2m} \frac{\partial^{2}}{\partial x_{2}^{2}} + \hat{V}(x_{2})$$
(12.24)

where

 $\hat{U}(x_1 - x_2)$ = the particle - particle interaction (12.25)

We will assume that $\hat{U}(x_1 - x_2)$ is small enough that we can apply perturbation theory. We then use direct product states and write

$$\hat{H} = \hat{H}_0 + \hat{U}$$
 (12.26)

$$\hat{H}_{1}\psi_{n_{1}}^{(0)}(x_{1}) = E_{n_{1}}^{(0)}\psi_{n_{1}}^{(0)}(x_{1})$$

$$\hat{H}_{1}\psi_{n_{1}}^{(0)}(x_{1}) = E_{n_{1}}^{(0)}\psi_{n_{1}}^{(0)}(x_{1})$$
(12.27)
$$\hat{H}_{1}\psi_{n_{1}}^{(0)}(x_{1}) = E_{n_{1}}^{(0)}\psi_{n_{1}}^{(0)}(x_{1})$$
(12.27)

$$\hat{H}_2\psi_{n_2}^{(0)}(x_2) = E_{n_2}^{(0)}\psi_{n_2}^{(0)}(x_2)$$
(12.28)

$$\hat{H}\psi_{n_{1}n_{2}}^{(0)}(x_{1},x_{2}) = \hat{H}_{0}\psi_{n_{1}}^{(0)}(x_{1})\psi_{n_{2}}^{(0)}(x_{2})$$

$$= (\hat{H}_{1} + \hat{H}_{2})\psi_{n_{1}}^{(0)}(x_{1})\psi_{n_{2}}^{(0)}(x_{2})$$

$$= (E_{n_{1}}^{(0)} + E_{n_{2}}^{(0)})\psi_{n_{1}}^{(0)}(x_{1})\psi_{n_{2}}^{(0)}(x_{2})$$

$$= E_{n_{1}n_{2}}^{(0)}\psi_{n_{1}n_{2}}^{(0)}(x_{1},x_{2})$$
(12.29)

We will construct the unperturbed (zero order) eigenfunctions and energies from these direct product states.

For the moment, we will also ignore spin.

The simple direct product states will not work for a description of the two particle system since the eigenfunctions of \hat{H}_0 must be either symmetric or antisymmetric under particle interchange.

The correct choice is ψ_S or ψ_A where

$$\psi_{n_1n_2}^{(0)S} = \frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) + \psi_{n_1}^{(0)}(x_2) \psi_{n_2}^{(0)}(x_1) \right]$$
(12.30)

$$\psi_{n_1n_2}^{(0)A} = \frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) - \psi_{n_1}^{(0)}(x_2) \psi_{n_2}^{(0)}(x_1) \right]$$
(12.31)

Both of these states have energy $E_{n_1n_2}^{(0)} = E_{n_1}^{(0)} + E_{n_2}^{(0)}$.

12.2 Bosons with Spin = 0

We assume that $s_1 = s_2 = 0$. This says that there are no new degrees of freedom and hence no reason to change the wave functions.

Indistinguishable bosons of spin = 0 require a symmetric wave function and thus we choose as the properly symmetrized zero-order wave functions

$$\psi_{n_1n_2}^{(0)S} = \frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) + \psi_{n_1}^{(0)}(x_2) \psi_{n_2}^{(0)}(x_1) \right]$$
(12.32)

The ground state corresponds to $n_1 = n_2 = 1$ or

$$\psi_{11}^{(0)S} = \psi_1^{(0)}(x_1)\psi_1^{(0)}(x_2)$$
(12.33)

In perturbation theory, the first order energy is then

$$E_{11} = 2E_{1}^{(0)} + \left\langle \psi_{11}^{(0)S} \middle| \hat{U}(x_{1} - x_{2}) \middle| \psi_{11}^{(0)S} \right\rangle$$

$$= 2E_{1}^{(0)}$$

$$+ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_{1} dx_{2} dx'_{1} dx'_{2}$$

$$\times \left\langle \psi_{11}^{(0)S} \middle| \left(\middle| \psi_{1}^{(0)}(x_{2}) \right\rangle \middle| \psi_{1}^{(0)}(x_{1}) \right\rangle \left\langle \psi_{1}^{(0)}(x_{1}) \middle| \left\langle \psi_{1}^{(0)}(x_{2}) \middle| \right) \right|$$

$$\times \hat{U}(x_{1} - x_{2}) \left(\middle| \psi_{1}^{(0)}(x'_{1}) \right\rangle \middle| \psi_{1}^{(0)}(x'_{2}) \right\rangle \left\langle \psi_{1}^{(0)}(x'_{1}) \middle| \left\langle \psi_{1}^{(0)}(x'_{2}) \middle| \right\rangle \middle| \psi_{11}^{(0)S} \right\rangle$$

$$(12.34)$$

Now

$$\left| \left\langle \psi_1^{(0)}(x_1) \right| \left\langle \psi_1^{(0)}(x_2) \right| \hat{U}(x_1 - x_2) \left| \psi_1^{(0)}(x_1') \right\rangle \left| \psi_1^{(0)}(x_2') \right\rangle$$

= $U(x_1 - x_2) \delta(x_1 - x_1') \delta(x_2 - x_2')$ (12.35)

which implies that

$$E_{11} = 2E_1^{(0)} + \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \left\langle \psi_{11}^{(0)S} \right| \left(\left| \psi_1^{(0)}(x_2) \right\rangle \left| \psi_1^{(0)}(x_1) \right\rangle \right) \\ \times U(x_1 - x_2) \left(\left\langle \psi_1^{(0)}(x_1) \right| \left\langle \psi_1^{(0)}(x_2) \right| \right) \left| \psi_{11}^{(0)S} \right\rangle$$
(12.36)

 or

$$E_{11} = 2E_1^{(0)} + \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \left| \psi_1^{(0)}(x_1) \right|^2 U(x_1 - x_2) \left| \psi_1^{(0)}(x_2) \right|^2$$
(12.37)

For later use we define the general direct integral

$$J_{n_1 n_2} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \left| \psi_{n_1}^{(0)}(x_1) \right|^2 U(x_1 - x_2) \left| \psi_{n_2}^{(0)}(x_2) \right|^2$$
(12.38)

In this case, we have

$$E_{11} = 2E_1^{(0)} + J_{11} \tag{12.39}$$

Now we look at the first excited state of this system. We assume that for the zero-order states, the first excited state corresponds to $n_1 = 1$ and $n_2 = 2$. Therefore, the zero-order symmetric wave function for the first excited state is

$$\psi_{12}^{(0)S} = \frac{1}{\sqrt{2}} \left[\psi_1^{(0)}(x_1) \psi_2^{(0)}(x_2) + \psi_1^{(0)}(x_2) \psi_2^{(0)}(x_1) \right]$$
(12.40)

and the first order energy is

$$E_{12} = E_1^{(0)} + E_2^{(0)} + \left\langle \psi_{12}^{(0)S} \right| \hat{U}(x_1 - x_2) \left| \psi_{12}^{(0)S} \right\rangle$$
(12.41)

Using the same procedure as before we get

$$E_{12} = E_1^{(0)} + E_2^{(0)} + J_{12} + K_{12}$$
(12.42)

where

$$K_{n_1n_2} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \psi_{n_1}^{(0)*}(x_1) \psi_{n_2}^{(0)}(x_1) U(x_1 - x_2) \psi_{n_2}^{(0)*}(x_2) \psi_{n_1}^{(0)}(x_2)$$
(12.43)

is called the *exchange integral*.

Now let us look at a possible physical meaning of these direct and exchange integrals.

We define

$$\left|\psi_{n_1}^{(0)}(x_1)\right|^2 = \rho_1 = \text{ probability density for particle 1 in state } n_1 \qquad (12.44)$$

and

$$\left|\psi_{n_2}^{(0)}(x_2)\right|^2 = \rho_2 = \text{ probability density for particle 2 in state } n_2 \qquad (12.45)$$

Therefore, the direct integrand takes the form

$$\rho_1 \rho_2 U(r_{12}) \tag{12.46}$$

To see what this means let

$$U(r_{12}) = \frac{e^2}{r_{12}} \tag{12.47}$$

which corresponds to a repulsive Coulomb potential. The direct integral is then

$$\int \int \frac{(e\rho_1)(e\rho_2)}{r_{12}} \, dx_1 \, dx_2 \tag{12.48}$$

This represents the total energy of two classical charge distributions interacting with the potential energy $U(r_{12})$.

The exchange integral, however, has no such classical counterpart. It is the result of symmetrizing the wave function and therefore arises because of the invariance of \hat{H} with respect to particle interchange.

The energy level diagram to first order might look like Figure 12.1 below.



Figure 12.1: Typical Boson Energy Level Diagram

The more interesting case is a two spin = 1/2 fermion system (since electrons are spin = 1/2 fermions).

12.3 Spin = 1/2 Fermions

The particles now have internal degrees of freedom. The single particle state vectors must now have both spatial and spin parts

$$|space\rangle|spin\rangle$$
 (12.49)

For example,

$$\left|\psi_{n_1}^{(0)}\right\rangle\left|+\right\rangle_1\tag{12.50}$$

presents a fermion in the $\psi_{n_1}^{(0)}$ spatial state with spin up.

We write the corresponding wave function as

$$\langle x_1 | \psi_{n_1}^{(0)} \rangle | + \rangle_1 = \psi_{n_1}^{(0)}(x_1)\alpha(1)$$
 (12.51)

and so on, where we define the labels $\alpha(j) = |+\rangle_j$ and $\beta(j) = |-\rangle_j$.

We must choose the antisymmetric combination for the zero-order wave func-

tions. We have 4 possible direct product states given n_1 and n_2 , i.e.,

$$\psi_1(1,2) = \psi_{n_1}^{(0)}(x_1)\psi_{n_2}^{(0)}(x_2)\alpha(1)\alpha(2)$$
(12.52)

$$\psi_2(1,2) = \psi_{n_1}^{(0)}(x_1)\psi_{n_2}^{(0)}(x_2)\alpha(1)\beta(2)$$
(12.53)

$$\psi_3(1,2) = \psi_{n_1}^{(0)}(x_1)\psi_{n_2}^{(0)}(x_2)\beta(1)\alpha(2)$$
(12.54)

$$\psi_4(1,2) = \psi_{n_1}^{(0)}(x_1)\psi_{n_2}^{(0)}(x_2)\beta(1)\beta(2)$$
(12.55)

These are not antisymmetric, however. A useful operator allows us to construct antisymmetric states. Consider the operator

$$\hat{R} = \frac{1}{\sqrt{2}} (1 - \hat{P}_{12}) \tag{12.56}$$

Now for any function A(1,2) we have

$$\hat{R}A(1,2) = \frac{1}{\sqrt{2}} (1 - \hat{P}_{12}) A(1,2) = \frac{1}{\sqrt{2}} [A(1,2) - A(2,1)]$$
(12.57)

which is antisymmetric. The factor $1/\sqrt{2}$ keeps the state normalized. We now use \hat{R} to construct four antisymmetric states from the four direct product states (12.52).

$$\psi_{n_1n_2++}^{(0)}(x_1, x_2) = \frac{1}{\sqrt{2}} (1 - \hat{P}_{12}) \psi_1(1, 2)$$

= $\frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) \alpha(1) \alpha(2) - \psi_{n_2}^{(0)}(x_1) \psi_{n_1}^{(0)}(x_2) \alpha(1) \alpha(2) \right]$ (12.58)

$$\psi_{n_{1}n_{2}+-}^{(0)}(x_{1},x_{2}) = \frac{1}{\sqrt{2}}(1-\hat{P}_{12})\psi_{2}(1,2)$$
$$= \frac{1}{\sqrt{2}} \left[\psi_{n_{1}}^{(0)}(x_{1})\psi_{n_{2}}^{(0)}(x_{2})\alpha(1)\beta(2) - \psi_{n_{2}}^{(0)}(x_{1})\psi_{n_{1}}^{(0)}(x_{2})\alpha(2)\beta(1)\right] \quad (12.59)$$

$$\psi_{n_1n_2-+}^{(0)}(x_1, x_2) = \frac{1}{\sqrt{2}} (1 - \hat{P}_{12}) \psi_3(1, 2)$$
$$= \frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) \beta(1) \alpha(2) - \psi_{n_2}^{(0)}(x_1) \psi_{n_1}^{(0)}(x_2) \alpha(1) \beta(2) \right] \quad (12.60)$$

$$\psi_{n_{1}n_{2}--}^{(0)}(x_{1},x_{2}) = \frac{1}{\sqrt{2}}(1-\hat{P}_{12})\psi_{4}(1,2)$$
$$= \frac{1}{\sqrt{2}} \left[\psi_{n_{1}}^{(0)}(x_{1})\psi_{n_{2}}^{(0)}(x_{2})\beta(1)\beta(2) - \psi_{n_{2}}^{(0)}(x_{1})\psi_{n_{1}}^{(0)}(x_{2})\beta(1)\beta(2)\right] \quad (12.61)$$

where the subscripts imply

- + + means both spins up
- + or + means one spin up and one spin down
- - means both spins down

Each of these wave functions is antisymmetric and each is an eigenfunction of \hat{H}_0 (since \hat{H}_0 does not contain any spin dependent terms) with the same energy. This implies that, at this point, we have a 4-fold degenerate zero-order system with energy $E_{n_1}^{(0)} + E_{n_2}^{(0)}$.

We could use these states as the zero-order wave function to start perturbation theory. It would be like doing the spin-orbit calculation using the $|\ell sm_\ell m_s\rangle$ basis, rather than the $|\ell sjm_j\rangle$ basis where \hat{H}_{so} is diagonal. It is always important to choose zero-order wave functions, if it is not to difficult to do, that incorporate as much of the symmetry of the system as possible. In other words, choose zero-order wave functions that are simultaneous eigenstates of the maximal set of commuting observables. This will hopefully produce a diagonal perturbation matrix or at least so many zeros that it is easy to diagonalize the rest of the matrix.

In this case, we not only have $[\hat{H}, \hat{P}_{12}] = 0$ which told us to choose antisymmetric zero-order states, but we also have $[\hat{H}, \vec{S}_{op}^2] = 0$ and $[\hat{H}, \hat{S}_z] = 0$ where

 $\vec{S}_{op} = \vec{S}_{1,op} + \vec{S}_{2,op} =$ the total spin angular momentum $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z} =$ the z - component of the total spin angular momentum

Therefore we should choose antisymmetric state functions which are also eigenfunctions of \hat{H}_0 , \vec{S}_{op}^2 and \hat{S}_z as our zero-order states.

From our earlier work we know that the possible values of the total spin are S = 0, 1 and the state vectors that are eigenstates of \vec{S}_{op}^2 and \hat{S}_z are

$$|1,1\rangle = \alpha(1)\alpha(2) = \chi_{11} \tag{12.62}$$

$$1,0\rangle = \frac{1}{\sqrt{2}} \left(\alpha(1)\beta(2) + \alpha(2)\beta(1) \right) = \chi_{10}$$
(12.63)

$$|1, -1\rangle = \beta(1)\beta(2) = \chi_{1, -1}$$
(12.64)

$$|0,0\rangle = \frac{1}{\sqrt{2}} \left(\alpha(1)\beta(2) - \alpha(2)\beta(1) \right) = \chi_{00}$$
(12.65)

Notice that the $\chi_{1,m=\pm 1,0}$ are symmetric under \hat{P}_{12} and χ_{00} is antisymmetric.

Therefore, we will maintain overall antisymmetry by writing the wave functions as products of spatial wave function and spin functions such that the spatial function is symmetric when combined with χ_{00} and the spatial function is anti-symmetric when combined with $\chi_{1,m=\pm 1,0}$.

The symmetric spatial function is

$$\psi_{n_1n_2}^{(0)S} = \frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) + \psi_{n_1}^{(0)}(x_2) \psi_{n_2}^{(0)}(x_1) \right]$$
(12.66)

and the antisymmetric spatial function is

$$\psi_{n_1n_2}^{(0)A} = \frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) - \psi_{n_1}^{(0)}(x_2) \psi_{n_2}^{(0)}(x_1) \right]$$
(12.67)

The four zero-order wave functions, which are now eigenfunctions of \hat{P}_{12} , \hat{H}_0 , \vec{S}_{op}^2 and \hat{S}_z are then

$$\psi_{n_1 n_2 00}^{(0)} = \frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) + \psi_{n_1}^{(0)}(x_2) \psi_{n_2}^{(0)}(x_1) \right] \chi_{00}$$
(12.68)

$$\psi_{n_1 n_2 1 m_s}^{(0)} = \frac{1}{\sqrt{2}} \left[\psi_{n_1}^{(0)}(x_1) \psi_{n_2}^{(0)}(x_2) - \psi_{n_1}^{(0)}(x_2) \psi_{n_2}^{(0)}(x_1) \right] \chi_{1 m_s} \quad m_s = \pm 1, 0$$
(12.69)

Notice that if we have identical spatial states, i.e., $n_1 = n_2$, the S = 1 states vanish identically. This says that two fermions in an S = 1 spin state cannot be in the same spatial state(the wavefunction vanishes). This is the first example of a general principle we will discuss later called the *Pauli Exclusion Principle*.

An alternative way to find these zero-order wave functions is to go back to first principles and use CG coefficients. For example

$$\psi_{n_1 n_2 s m_s}^{(0)} = \sum_{\substack{m_{s_1}, m_{s_2} \\ m_{s_1} + m_{s_2} = m_s}} a_{m_{s_1}, m_{s_2}} \psi_{n_1 n_2 m_{s_1} m_{s_2}}^{(0)}$$
(12.70)

where

$$a_{m_{s_1}m_{s_2}} = \langle s_1 s_2 m_{s_1} m_{s_2} \mid s_1 s_2 s m_s \rangle \tag{12.71}$$

Now

$$\left\langle \frac{1}{2} \frac{1}{2} m_{s_1} m_{s_2} \left| \frac{1}{2} \frac{1}{2} 11 \right\rangle = \delta_{m_{s_1}, \frac{1}{2}} \delta_{m_{s_2}, \frac{1}{2}}$$
(12.72)

which implies that

$$\psi_{n_1 n_2 11}^{(0)} = \psi_{n_1 n_2 + +}^{(0)} \tag{12.73}$$

as written above.

Similarly, for $s = 1, m_s = 0$, the only nonzero CG coefficients are

$$\left(\frac{1}{2}\frac{1}{2}\frac{1}{2} - \frac{1}{2}\left|\frac{1}{2}\frac{1}{2}10\right\rangle = \frac{1}{\sqrt{2}} = \left(\frac{1}{2}\frac{1}{2} - \frac{1}{2}\frac{1}{2}\left|\frac{1}{2}\frac{1}{2}10\right\rangle$$
(12.74)

which implies that

$$\psi_{n_{1}n_{2}10}^{(0)} = \frac{1}{\sqrt{2}}\psi_{n_{1}n_{2}+-}^{(0)} + \frac{1}{\sqrt{2}}\psi_{n_{1}n_{2}-+}^{(0)}$$
$$= \frac{1}{\sqrt{2}} \left[\psi_{n_{1}}^{(0)}(1)\psi_{n_{2}}^{(0)}(2) - \psi_{n_{1}}^{(0)}(2)\psi_{n_{2}}^{(0)}(1)\right]\chi_{10}$$
(12.75)

as written above. We now have the appropriate zero-order wave functions and can apply perturbation theory to the two fermion system.

As with the two boson case, the zero-order ground state for two fermions corresponds to $n_1 = n_2 = 1$ with zero-order energy $2E_1^{(0)}$. Since the S = 1 or triplet states have identically zero state functions in the case (since the spatial function are antisymmetric), we have $\psi_{11,1m_s}^{(0)} = 0$. The unperturbed ground state must then have $S = 0, S_z = 0$ or it is $\psi_{11,00}^{(0)}(1,2)$. This involves a singlet state with $m_s = 0$ only

$$\chi_{00} = \frac{1}{\sqrt{2}} \left(\alpha(1)\beta(2) - \beta(1)\alpha(2) \right)$$
(12.76)

In this state, the particle spins are always opposite or antiparallel.

The ground state energy to first order is

$$E_{11} = 2E_1^{(0)} + \left| \psi_{11,00}^{(0)} \right| \hat{U}(x_1 - x_2) \left| \psi_{11,00}^{(0)} \right|$$
$$= 2E_1^{(0)} + J_{11}$$
(12.77)

which is the *same* energy as in the two boson system(we are assuming the *same Hamiltonian* applies).

The spatial part of the wave function is the same also, namely,

$$\psi_1^{(0)}(1)\psi_2^{(0)}(2) \tag{12.78}$$

We must use a symmetric spatial wave function here because the spin vector is antisymmetric in the ground state of two fermions. The presence of the spin internal degrees of freedom(and the Pauli principle) has a more dramatic effect on the first excited state for two fermions.

We again assume that the first excited state corresponds to $n_1 = 1, n_2 = 2$. This gives the energy to first order as

$$E_{12} = E_1^{(0)} + E_2^{(0)} + \left(\psi_{12,sm_s}^{(0)} \middle| \hat{U}(x_1 - x_2) \middle| \psi_{12,sm_s}^{(0)} \right)$$
(12.79)

We can write the energy this way, i.e., we do not need to write a 4×4 matrix $\langle \hat{U} \rangle$ and diagonalize it because the $\langle \hat{U} \rangle$ matrix is already diagonal in this basis due the orthogonality of the spin functions and the fact that the perturbing potential does not depend on spin. This first order energy is different for the triplet and singlet states. If we do the integrals (they are the same as the boson case) we get

$$E_{12} = E_1^{(0)} + E_2^{(0)} + J_{12} \pm K_{12}$$
(12.80)

where

$$+ \rightarrow \text{ singlet } s = 0, m_s = 0$$

 $- \rightarrow \text{ triplet } s = 1, m_s = \pm 1, 0$
All the triplet states have the same energy because they have the same spatial wave function and the perturbing potential does not depend on spin.

We thus get the energy level structure shown in Figure 12.2 below.



Figure 12.2: Typical Fermion Energy Level Diagram

The energies now depend on the total spin S even though the Hamiltonian \hat{H} does not explicitly depend on spin. A very dramatic effect!!

This level splitting is not due to any additional terms added to the Hamiltonian such as \hat{H}_{so} or \hat{H}_{Zeeman} . This effect is strictly due to symmetry requirements. The requirement of symmetry or antisymmetry forced on the spatial wave functions by the symmetry or antisymmetry of the spin vectors causes this level splitting. The entire effect is due to the invariance of the Hamiltonian under pairwise particle interchange.

Physically, we can argue as follows:

- 1. symmetric spatial functions are large for $x_1\approx x_2$, while antisymmetric spatial functions are ≈ 0 for $x_1\approx x_2$
- 2. $U(x_1 x_2)$ is expected to be largest for $x_1 \approx x_2$
- 3. this implies that for S = 1 fermions $\langle \hat{U} \rangle$ is relatively small while for S = 0 fermions $\langle \hat{U} \rangle$ is relatively large
- 4. two identical fermions with antiparallel spins have a large probability of being close together they *attract* each other
- 5. two identical fermions with parallel spins have zero probability of being close together they *repel* each other

This *repulsion* is spin dependent and not due to the Coulomb repulsion between the electrons.

The first order energy for the singlet state is larger than for the triplet states because the repulsive interaction is enhanced in the singlet state. This overall effect is called *spin pairing* and it is a purely quantum mechanical effect.

12.4 The N-Electron Atom

We now extend our discussion to a system with N electrons (fermions). We write

$$\hat{H} = \hat{H}_0 + \hat{H}' \tag{12.81}$$

where

$$\hat{H}_0 = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m_e} \nabla_i^2 + \hat{V}(\vec{r}_i) \right]$$
(12.82)

$$\hat{H}' = \sum_{i=1}^{N} \sum_{j>i}^{N} \hat{U}(\vec{r}_i - \vec{r}_j)$$
(12.83)

The energy eigenstates for the N-electron atom are solutions of the time independent Schrödinger equation

$$\hat{H}\psi_E = E\psi_E \tag{12.84}$$

where $\psi_E = \psi_E(1, 2, 3, 4, ..., N)$ and $1 = (\vec{r}_1, s_1)$ and so on.

The indistinguishability of the N electrons implies that

$$\left[\hat{H}, \hat{P}_{ij}\right] = 0 \qquad i, j = 1, 2, 3, 4, \dots, N \ ; \ i \neq j \tag{12.85}$$

where the \hat{P}_{ij} interchange all attributes of the electrons, i.e., both the spatial and spin degrees of freedom.

The wave function must be antisymmetric under pairwise electron interchange

$$\hat{P}_{ij}\psi_E = -\psi_E \qquad i, j = 1, 2, 3, 4, \dots, N \; ; \; i \neq j \tag{12.86}$$

The general problem of N interacting electrons is very complex. At this stage we only want to extract general properties that will also hold in real 3-dimensional atomic systems. It turns out to be instructive to consider the case of non-interacting electrons - the so-called independent particle model. In this model we neglect the electron-electron interactions and look only at the zeroth order.

In particular, we consider N identical non-interacting particles in a potential well $V(\vec{r})$. The Hamiltonian for any particle in the well is

$$\hat{H}_0(k) = \frac{\vec{p}_{k,op}^2}{2m} + V(\vec{r}_k)$$
(12.87)

where

$$\hat{H}_0(k)\phi_n(\vec{r}_k) = \varepsilon_n\phi_n(\vec{r}_k) \qquad n = 0, 1, 2, 3, 4, \dots$$
 (12.88)

Thus, any single particle sees the energy level structure as shown in Figure 12.3 below.



Figure 12.3: Single Particle Energy Level Structure

The N-particle Hamiltonian is then

$$\hat{H} = \hat{H}_0(1) + \hat{H}_0(2) + \hat{H}_0(3)..... + \hat{H}_0(N)$$
(12.89)

with solutions given by

$$\hat{H}\psi(1,2,3,...,N) = E\psi(1,2,3,...,N)$$
 (12.90)

where

$$\psi(1,2,3,...,N) = \phi_a(1)\phi_b(2)...,\phi_n(N)$$
(12.91)

and

$$E = \varepsilon_a + \varepsilon_b + \dots + \varepsilon_n \tag{12.92}$$

This solution implies that

```
particle 1 is in state a with energy \varepsilon_a
particle 2 is in state b with energy \varepsilon_b
.....
particle N is in state n with energy \varepsilon_n
```

Electrons have spin = 1/2. Thus, corresponding to any single particle energy level, say a, there are two possible single particle states, namely,

$$\phi_a(1)\alpha(1) \text{ and } \phi_a(1)\beta(1)$$
 (12.93)

From now on when we write $\phi_a(1)$, where the subscript *a* will be understood to also include the spin information.

The simple product state solutions are not physically admissible solutions since

they are not antisymmetric under particle interchange for any two particles.

All such states with particles interchanged pairwise have the same energy. In fact, any permutation of the indices produces a state with the same energy. We need to construct a completely antisymmetric linear combination of all of these solutions.

If these were bosons we would have to construct a completely symmetric linear combination of all these solutions.

If we define

$$\wp \psi(1,2,3,4,\ldots,N) = a \text{ permutation of the particles}$$
 (12.94)

then, the completely symmetric state is easy to construct. It is

$$\psi_S(1,2,3,...,N) = \sum_{\wp} \wp \psi(1,2,3,4,...,N)$$
 (12.95)

where the sum means a sum over all possible permutations or arrangements. There are N! such permutations.

Examples

$$N = 2 \rightarrow N! = 2$$

$$\psi_{S}(1,2) = \phi_{1}(1)\phi_{2}(2) + \phi_{1}(2)\phi_{2}(1)$$

$$N = 3 \rightarrow N! = 6$$

$$\psi_{S}(1,2,3) = \phi_{1}(1)\phi_{2}(2)\phi_{3}(3) + \phi_{1}(2)\phi_{2}(1)\phi_{3}(3) + \phi_{1}(3)\phi_{2}(2)\phi_{3}(1)$$

$$+ \phi_{1}(1)\phi_{2}(3)\phi_{3}(2) + \phi_{1}(3)\phi_{2}(1)\phi_{3}(2) + \phi_{1}(2)\phi_{2}(3)\phi_{3}(1)$$

How do we construct a completely antisymmetric state? Let us define a general permutation operator by (illustrate for N = 5)

$$\hat{\wp}_{13452}\psi(1,2,3,4,5) = \psi(3,1,4,5,2)$$
$$\hat{\wp}_{23451}\psi(1,2,3,4,5) = \psi(2,3,4,5,1)$$

Any such permutation operator can be written as the product of the 2-particle interchange operators \hat{P}_{ij} , i.e.,

$$\psi(2,3,1) = \hat{\wp}_{231}\psi(1,2,3)$$
$$= \hat{P}_{12}\psi(3,2,1) = \hat{P}_{12}\hat{P}_{13}\psi(1,2,3)$$

Thus, any permutation $\hat{\wp}$ can be written in terms of an odd or even number of pair interchanges or pair permutations and we call it an odd or even permutation accordingly. All pair permutations are odd.

Therefore, for a completely antisymmetric state we must have

$$\hat{\wp}\psi_A = \begin{cases} +\psi_A & \text{if } \hat{\wp} \text{ is an even permutation} \\ -\psi_A & \text{if } \hat{\wp} \text{ is an odd permutation} \end{cases}$$
(12.96)

We therefore form a completely antisymmetric state as follows. We let

$$(-1)^{\hat{\wp}} = \begin{cases} +1 & \text{if } \hat{\wp} \text{ is an even permutation} \\ -1 & \text{if } \hat{\wp} \text{ is an odd permutation} \end{cases}$$
(12.97)

and then

Examples

$$\begin{split} N &= 2 \rightarrow N! = 2 \\ \psi_A(1,2) &= \phi_1(1)\phi_2(2) - \phi_1(2)\phi_2(1) \\ N &= 3 \rightarrow N! = 6 \\ \psi_A(1,2,3) &= \phi_1(1)\phi_2(2)\phi_3(3) - \phi_1(2)\phi_2(1)\phi_3(3) - \phi_1(3)\phi_2(2)\phi_3(1) \\ &- \phi_1(1)\phi_2(3)\phi_3(2) + \phi_1(3)\phi_2(1)\phi_3(2) + \phi_1(2)\phi_2(3)\phi_3(1) \end{split}$$

It is clear that if any two states are identical (put 2 = 3 above), then ψ_A is identically = 0 as it should be for fermions.

This implies that we can put at most 2 electrons in each energy level of the potential well. The two electrons in the k^{th} level would then have wave functions

$$\phi_k \alpha \text{ and } \phi_k \beta$$
 (12.98)

i.e., they must have opposite spins. This says that N spin = 1/2 fermions must occupy at least N/2 different states in the well.

This is very different than for bosons where all the N bosons can be in any energy level.

Another way to write the completely antisymmetric wave function for fermions is the so-called Slater determinant

$$\psi_A(1,2,3,...,N) = \begin{vmatrix} \phi_a(1) & \phi_a(2) & ... & \phi_a(N) \\ \phi_b(1) & \phi_b(2) & ... & \phi_b(N) \\ ... & ... & ... \\ \phi_n(1) & \phi_n(2) & ... & \phi_n(N) \end{vmatrix}$$
(12.99)

The last thing we must do is to normalize these state vectors.

$$\begin{aligned} \langle \psi_A \, | \, \psi_A \rangle &= \sum_{s_1, s_2, \dots, s_N} \int d^3 \vec{r}_1 \dots d^3 \vec{r}_N \\ &\times \sum_{\wp \wp'} (-1)^{\wp} (-1)^{\wp'} [\wp \phi_a^*(1) \dots \phi_n^*(N)] [\wp' \phi_a(1) \dots \phi_n(N)] \end{aligned}$$

Now if $\wp \neq \wp'$, then $[\wp \phi_a(1)...,\phi_n(N)]$ and $[\wp' \phi_a(1)...,\phi_n(N)]$ are orthogonal and the integration for that term is zero.

Therefore, we get

$$\langle \psi_A | \psi_A \rangle = \sum_{s_1, s_2, \dots, s_N} \int d^3 \vec{r}_1 \dots d^3 \vec{r}_N \sum_{\wp} \wp |\phi_a(1)|^2 \dots |\phi_n(N)|^2 \qquad (12.100)$$

But

$$\sum_{s_k} \int d^3 \vec{r}_k \left| \phi_k(j) \right|^2 = 1$$
 (12.101)

so we finally get

$$\langle \psi_A \mid \psi_A \rangle = \sum_{\wp} 1 = \text{ number of possible permutations } = N!$$
 (12.102)

and therefore, the properly normalized completely antisymmetric wave function is $| f_{ij} = f_{ij} =$

$$\psi_A(1,2,3,...,N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_a(1) & \phi_a(2) & . & \phi_a(N) \\ \phi_b(1) & \phi_b(2) & . & \phi_b(N) \\ . & . & . & . \\ \phi_n(1) & \phi_n(2) & . & \phi_n(N) \end{vmatrix}$$
(12.103)

In a similar manner

$$\langle \psi_S \mid \psi_S \rangle = \frac{N!}{N_a!....N_n!} \tag{12.104}$$

where

 N_k = the number of times the single particle state ϕ_k occurs

What is the difference between the ground state of N fermions and N bosons?

For N bosons, all N particles occupy the lowest level ϕ_0 and the wavefunction is

$$\psi_S(1,2,3,\dots,N) = \phi_0(1)\phi_0(2)\phi_0(3)\dots\phi_0(N)$$
(12.105)

with energy

$$E_0 = N\varepsilon_0 \tag{12.106}$$

This is true no matter how large N might be, even for macroscopic systems where $N \approx 10^{23}$. As we shall see in later discussions, this is one of the physical requirements for phenomena like superconductivity, superfluidity and Bose-Einstein condensation.

Such a state is not allowed for fermions however. We must have

| N even | N odd |
|--------------------------------------|--------------------------------------|
| $2 \text{ in } \phi_0$ | $2 \text{ in } \phi_0$ |
| $2 \text{ in } \phi_1$ | $2 \text{ in } \phi_1$ |
| | |
| $2 \text{ in } \phi_{\frac{N}{2}-1}$ | $2 \text{ in } \phi_{\frac{N-1}{2}}$ |
| $2 \text{ in } \phi_{\frac{N}{2}}$ | 1 in $\phi_{\frac{N+1}{2}}$ |

This difference for systems with even or odd numbers of fermions will lead to dramatic physical consequences later for some atomic systems.

The ground state energy for N fermions is

| $2(\varepsilon_0 + \varepsilon_1 + \dots + \varepsilon_{\frac{N}{2}})$ | for N even |
|--|--------------|
| $2(\varepsilon_0 + \varepsilon_1 + \dots + \varepsilon_{\frac{N-1}{2}}) + \varepsilon_{\frac{N+1}{2}}$ | for N odd |

Either of these two energies is always greater than the N boson ground state energy.

The extra energy is called the *zero point energy* and it arises from particle interchange invariance or it arises from the *Pauli Exclusion Principle* which states

No two identical fermions in a physical system can have the same set of quantum numbers

It is equivalent to the antisymmetry of the wave function requirement for fermions.

12.5 The Helium Atom

We now consider the simplest multielectron atom, namely, helium, which has two electrons. The Hamiltonian is

$$\hat{H} = \hat{H}(1) + \hat{H}(2) + \hat{V} = \frac{\vec{p}_{1,op}^2}{2m} - \frac{Ze^2}{r_1} + \frac{\vec{p}_{2,op}^2}{2m} - \frac{Ze^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$
(12.107)

where

 $\hat{H}(i)$ = hydrogen atom Hamiltonian with nuclear charge Ze (instead of e)

 \hat{V} = electrostatic repulsion between the electrons

We start by neglecting the electrostatic repulsion between the electrons. This gives us a zero-order solution that we can use in perturbation theory. This is equivalent to the independent particle model we just discussed.

Since $\hat{H} = \hat{H}(1) + \hat{H}(2)$ in this model, we can write

$$|\psi\rangle = |n_1\ell_1m_1\rangle |n_2\ell_2m_2\rangle \tag{12.108}$$

where

$$\hat{H}(1) |n_1 \ell_1 m_1\rangle = E_{n_1}^{(0)} |n_1 \ell_1 m_1\rangle \text{ and } \hat{H}(2) |n_2 \ell_2 m_2\rangle = E_{n_2}^{(0)} |n_2 \ell_2 m_2\rangle$$

$$\hat{H} |\psi\rangle = (\hat{H}(1) + \hat{H}(2)) |\psi\rangle = (\hat{H}(1) + \hat{H}(2)) |n_1 \ell_1 m_1\rangle |n_2 \ell_2 m_2\rangle$$

$$= E_{n_1 n_2}^{(0)} |\psi\rangle = (E_{n_1}^{(0)} + E_{n_2}^{(0)}) |n_1 \ell_1 m_1\rangle |n_2 \ell_2 m_2\rangle = (E_{n_1}^{(0)} + E_{n_2}^{(0)}) |\psi\rangle$$

and

$$E_n^{(0)} = -\frac{Z^2 e^2}{2a_0 n^2}$$
 (Z = 2 for helium) (12.109)

We will be working out the numbers in this problem so that we can compare our results to experiment. The zero order energies are shown in Table 12.1 below:

| n_1 | n_2 | $E_{n_1n_2}^{(0)}(Ry)$ | $E_{n_1n_2}^{(0)}(eV)$ |
|-------|-------|------------------------|------------------------|
| 1 | 1 | -8 | -108.8 |
| 1 | 2 | -5 | -68.0 |
| 1 | 3 | -40/9 | -64.4 |
| 1 | | | |
| 1 | | -4 | -54.5 |
| 2 | 2 | -2 | -27.2 |

Table 12.1: Zero Order Energies

where

1 Ry(Rydberg) =
$$\frac{e^2}{2a_0}$$
 = 13.6 eV (12.110)

The ground state energy is

$$E_{gs} = E_{11}^{(0)} = 2E_1^{(0)} = -8 Ry$$
(12.111)

and the energy of the system when one electron has been ionized (no longer bound) is

$$E_{ion} = E_1^{(0)} + E_{\infty}^{(0)} = -4 Ry \qquad (12.112)$$

Therefore, it requires the addition of 4 Ry to create singly ionized helium. Notice that the (2,2) state has an energy greater than E_{ion} , which implies that it is not a bound state of the helium atom. All the states (1,n) are bound states. The energy level spectrum looks as shown in Figure 12.4 below.



Figure 12.4: Helium Energy level Spectrum

Since the particles are electrons we must antisymmetrize the wave functions. We have two spin = 1/2 fermions. The spin functions are

$$|s, m_s\rangle = \begin{cases} |1, (\pm 1, 0)\rangle & \to \text{symmetric} \\ |0, 0\rangle & \to \text{antisymmetric} \end{cases}$$
(12.113)

The spatial part of the wave function must be of opposite symmetry to the spin functions so that the product is antisymmetric. By convention we label the states as follows:

Parahelium

$$(\text{symmetric space part})\chi_{00} \\ (|100\rangle |100\rangle) |00\rangle \\ \frac{1}{\sqrt{2}} [|100\rangle |2\ell m\rangle + |2\ell m\rangle |100\rangle] \chi_{00}$$

and so on.

Orthohelium

(antisymmetric space part)
$$\chi_{1m_s}$$

$$\frac{1}{\sqrt{2}} [|100\rangle |2\ell m\rangle - |2\ell m\rangle |100\rangle] \chi_{1m}$$

and so on.

These are the zero-order wave functions. We now handle the

$$\frac{e^2}{|\vec{r}_1 - \vec{r}_2|} = \frac{e^2}{r_{12}} \tag{12.114}$$

term by perturbation theory.

The first order ground state energy correction is

$$\Delta E = \langle 100 | \langle 100 | \frac{e^2}{r_{12}} | 100 \rangle | 100 \rangle \langle 00 | 00 \rangle$$
$$= e^2 \int \int d^3 \vec{r}_1 d^3 \vec{r}_2 \frac{|\psi_{100}(\vec{r}_1)|^2 |\psi_{100}(\vec{r}_2)|^2}{r_{12}}$$
(12.115)

where

$$\psi_{100}(\vec{r}) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Zr}{a_0}}$$
(12.116)

Therefore,

$$\Delta E = \frac{1}{\pi^2} \left(\frac{Z}{a_0}\right)^3 e^2 \int_0^\infty dr_1 r_1^2 e^{-\frac{2Zr_1}{a_0}} \int_0^\infty dr_2 r_2^2 e^{-\frac{2Zr_2}{a_0}} \int \int d\Omega_1 d\Omega_2 \frac{1}{r_{12}} \quad (12.117)$$

Even though this calculation does not give a very accurate result, it is still very instructive to learn the tricks necessary to evaluate the integrals.

We first need to find a useful expression for $1/r_{12}$. We have

$$r_{12} = |\vec{r}_1 - \vec{r}_2| = \sqrt{(\vec{r}_1 - \vec{r}_2) \cdot (\vec{r}_1 - \vec{r}_2)}$$
(12.118)

$$r_{12}^{2} = (\vec{r}_{1} - \vec{r}_{2}) \cdot (\vec{r}_{1} - \vec{r}_{2}) = r_{1}^{2} + r_{2}^{2} - 2\vec{r}_{1} \cdot \vec{r}_{2}$$
$$= r_{1}^{2} + r_{2}^{2} - 2r_{1}r_{2}\cos\beta \qquad (12.119)$$

where

$$\beta$$
 = angle between \vec{r}_1 and \vec{r}_2 (12.120)

Therefore,

$$\frac{1}{r_{12}} = \frac{1}{\left(r_1^2 + r_2^2 - 2r_1r_2\cos\beta\right)^{1/2}}$$
(12.121)

In the subsequent development, we let the larger of r_1,r_2 be called $r_>$ and the smaller be called $r_<.$ We then have

$$\frac{1}{r_{12}} = \frac{1}{r_{>} \left(1 - 2\frac{r_{<}}{r_{>}}\cos\beta + \left(\frac{r_{<}}{r_{>}}\right)^{2}\right)^{1/2}}$$
$$= \frac{1}{r_{>}} + \frac{1}{2r_{>}} \left(2\frac{r_{<}}{r_{>}}\cos\beta - \left(\frac{r_{<}}{r_{>}}\right)^{2}\right) - \frac{3}{8r_{>}} \left(2\frac{r_{<}}{r_{>}}\cos\beta - \left(\frac{r_{<}}{r_{>}}\right)^{2}\right)^{2}$$
$$+ \frac{15}{48r_{>}} \left(2\frac{r_{<}}{r_{>}}\cos\beta - \left(\frac{r_{<}}{r_{>}}\right)^{2}\right)^{3} - \dots$$
(12.122)

or

$$\frac{1}{r_{12}} = \frac{1}{r_{>}} \left[1 + \frac{r_{<}}{r_{>}} \cos\beta + \left(\frac{r_{<}}{r_{>}}\right)^{2} \left(\frac{3}{2}\cos^{2}\beta - \frac{1}{2}\right) + \dots \right]$$
(12.123)

$$= \frac{1}{r_{>}} \left[P_0(\cos\beta) + \frac{r_{<}}{r_{>}} P_1(\cos\beta) + \left(\frac{r_{<}}{r_{>}}\right)^2 P_2(\cos\beta) + \dots \right]$$
(12.124)

Therefore,

$$\frac{1}{r_{12}} = \frac{1}{r_{>}} \sum_{\lambda=0}^{\infty} \left(\frac{r_{<}}{r_{>}}\right)^{\lambda} P_{\lambda}(\cos\beta)$$
(12.125)

Now, the addition theorem for spherical harmonics, which is proved at the end of this chapter, gives

$$P_{\lambda}(\cos\beta) = \frac{4\pi}{2\lambda + 1} \sum_{m=-\lambda}^{\lambda} Y_{\lambda m}(\Omega_1) Y_{\lambda m}^*(\Omega_2)$$
(12.126)

Therefore, we finally have

$$\frac{1}{r_{12}} = \frac{1}{r_{>}} \sum_{\lambda=0}^{\infty} \left(\frac{r_{<}}{r_{>}}\right)^{\lambda} \frac{4\pi}{2\lambda+1} \sum_{m=-\lambda}^{\lambda} Y_{\lambda m}(\Omega_{1}) Y_{\lambda m}^{*}(\Omega_{2})$$
(12.127)

Now, the factor

$$\int \int d\Omega_1 d\Omega_2 \frac{1}{r_{12}} \tag{12.128}$$

contains terms like

$$\int \int d\Omega_1 d\Omega_2 Y_{\lambda m}(\Omega_1) Y^*_{\lambda m}(\Omega_2)$$
(12.129)

and

$$\int d\Omega Y_{\lambda m}(\Omega) \propto \int d\Omega Y_{\lambda m}(\Omega) Y_{00}(\Omega) = \delta_{\lambda 0} \delta_{m0} \qquad (12.130)$$

Therefore, the only term that contributes from the sum is $\lambda = m = 0$ and we get

$$\int \int d\Omega_1 d\Omega_2 \frac{1}{r_{12}} = \frac{1}{r_{>}}$$
(12.131)

and therefore we have

$$\Delta E = \frac{1}{\pi^2} \left(\frac{Z}{a_0}\right)^3 e^2 \int_0^\infty dr_1 r_1^2 e^{-\frac{2Zr_1}{a_0}} \int_0^\infty dr_2 r_2^2 e^{-\frac{2Zr_2}{a_0}} \frac{1}{r_>}$$
(12.132)

or

$$\Delta E = \frac{1}{\pi^2} \left(\frac{Z}{a_0}\right)^3 e^2 \int_0^\infty dr_1 r_1^2 e^{-\frac{2Zr_1}{a_0}} \int_0^{r_1} dr_2 r_2^2 e^{-\frac{2Zr_2}{a_0}} \frac{1}{r_1} + \frac{1}{\pi^2} \left(\frac{Z}{a_0}\right)^3 e^2 \int_0^\infty dr_1 r_1^2 e^{-\frac{2Zr_1}{a_0}} \int_{r_1}^\infty dr_2 r_2^2 e^{-\frac{2Zr_2}{a_0}} \frac{1}{r_2}$$
(12.133)

which gives

$$\Delta E = \frac{5}{8} \frac{Ze^2}{a_0} = J_{1s,1s} = J_{10,10} = 2.5 \ Ry = 34 \ eV \tag{12.134}$$

for Z = 2.

The ground state energy corrected to first order is then

$$E_{11} = E_{11}^{(0)} + \Delta E = -74.8 \ eV = -5.5 \ Ry \tag{12.135}$$

The experimental value is

$$(E_{11})_{\exp t} = -78.975 \ eV = -5.807 \ Ry \tag{12.136}$$

This first order result is amazingly good for this complex system!

Now we deal with the first excited state.

The first order energy shifts are once again given by standard perturbation theory since the $\langle \hat{V} \rangle$ matrix is diagonal in this basis due to the orthonormality of the spin vectors and the fact that \hat{V} is independent of spin.

We thus have

$$\Delta E_{n\ell}^{s,t} = \frac{1}{2} \int \int d^3 \vec{r}_1 d^3 \vec{r}_2 \left| \psi_{100}(1) \psi_{n\ell 0}(2) \pm \psi_{100}(2) \psi_{n\ell 0}(1) \right|^2 \frac{e^2}{r_{12}} \quad (12.137)$$

where $s, t \rightarrow \text{singlet}$, triplet $\rightarrow S = 0, 1 \rightarrow -, +$. As shown before, we need only calculate the m = 0 case because $[\vec{L}_{op}, \hat{V}] = 0$ where

$$\vec{L}_{op} = \vec{L}_{1,op} + \vec{L}_{2,op} = \text{ total orbital angular momentum}$$
(12.138)

which implies that the result is independent of m.

Therefore

$$\Delta E_{n\ell}^{s,t} = e^2 \int \int d^3 \vec{r}_1 d^3 \vec{r}_2 \left| \psi_{100}(1) \right|^2 \left| \psi_{n\ell 0}(2) \right|^2 \frac{1}{r_{12}}$$

$$+ e^2 \int \int d^3 \vec{r}_1 d^3 \vec{r}_2 \psi_{100}^*(1) \psi_{n\ell 0}^*(2) \psi_{100}(2) \psi_{n\ell 0}(1) \frac{1}{r_{12}} = J_{n\ell} \pm K_{n\ell}$$
(12.139)

where

$$J_{n\ell}$$
 = electrostatic repulsion between two charge distributions
 $|\psi_{100}(1)|^2$ and $|\psi_{n\ell 0}(2)|^2$ = the direct integral

and

 $K_{n\ell}$ = the exchange integral which arises from antisymmetrization of the wave function

with

$$+ =$$
singlet and $- =$ triplet

A convenient way of representing this result is as follows.

$$\vec{S}_{op} = \vec{S}_{1,op} + \vec{S}_{2,op}$$

$$\rightarrow 2\vec{S}_{1,op} \cdot \vec{S}_{2,op} = \vec{S}_{op}^2 - \vec{S}_{1,op}^2 - \vec{S}_{2,op}^2 = \hbar^2 (S(S+1) - \frac{3}{2})$$
(12.140)

$$2\vec{S}_{1,op} \cdot \vec{S}_{2,op} = \hbar^2 \begin{cases} +\frac{1}{2} & \text{triplet} \\ -\frac{3}{2} & \text{singlet} \end{cases}$$
(12.141)

and therefore

$$\Delta E_{n\ell}^{s,t} = J_{n\ell} - \frac{1}{2\hbar^2} (1 + 4\vec{S}_{1,op} \cdot \vec{S}_{2,op}) K_{n\ell}$$
(12.142)

The calculation results (in eV) are shown in Table 12.2 below and the energy levels are shown in Figure 12.5 below. Not bad!!

| State | 1s2s | | 1s2p | |
|----------------|---------------|---------------|---------------|------------|
| $n\ell$ | 10,20 | 10,20 | 10,21 | 10,21 |
| | singlet | triplet | singlet | triplet |
| 0^{th} order | -68.0 | -68.0 | -68.0 | -68.0 |
| J | 11.4 | 11.4 | 13.2 | 13.2 |
| K | 1.2 | 1.2 | 0.9 | 0.9 |
| 1^{st} order | -55.4 | -57.8 | -53.9 | -55.7 |
| E_{expt} | -58.4 | -59.2 | -57.8 | -58.0 |
| error | $3.0{=}5.1\%$ | $1.4{=}2.4\%$ | $3.9{=}6.7\%$ | 2.3 = 4.0% |

 Table 12.2: Calculation Results



Figure 12.5: Helium Energy Levels

For comparison, we will also calculate the ground state energy using the variational method. We neglect spin in this case. The simplest choice of a trial function is the product of two hydrogen atom wave functions as in (12.143) below, which would be an exact solution if the electron-electron repulsion was neglected.

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Zr_1}{a_0}} \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Zr_2}{a_0}}$$
(12.143)

Since we expect the true wave function to be approximately represented by the above function, we change Z to α and thus obtain the best possible value for E_0 for this type of trial function.

We do the calculation as follows. We write

$$\hat{H} = \hat{H}_{Z}(1) + \hat{H}_{Z}(2) + \hat{V} = \frac{\vec{p}_{1,op}^{2}}{2m} - \frac{Ze^{2}}{r_{1}} + \frac{\vec{p}_{2,op}^{2}}{2m} - \frac{Ze^{2}}{r_{2}} + \frac{e^{2}}{r_{12}}$$

$$= \frac{\vec{p}_{1,op}^{2}}{2m} - \frac{\alpha e^{2}}{r_{1}} + \frac{\vec{p}_{2,op}^{2}}{2m} - \frac{\alpha e^{2}}{r_{2}} + \frac{(\alpha - Z)e^{2}}{r_{1}} + \frac{(\alpha - Z)e^{2}}{r_{2}} + \frac{e^{2}}{r_{12}}$$

$$= \hat{H}_{\alpha}(1) + \hat{H}_{\alpha}(2) + \frac{(\alpha - Z)e^{2}}{r_{1}} + \frac{(\alpha - Z)e^{2}}{r_{2}} + \frac{e^{2}}{r_{12}}$$
(12.144)

Now

$$\hat{H}_{\alpha}(1)\psi_{100}^{\alpha}(1) = E_{100}^{(0)}(\alpha)\psi_{100}^{\alpha}(1) = -\alpha^{2}\psi_{100}^{\alpha}(1)$$
(12.145)

$$\hat{H}_{\alpha}(2)\psi_{100}^{\alpha}(2) = E_{100}^{(0)}(\alpha)\psi_{100}^{\alpha}(2) = -\alpha^{2}\psi_{100}^{\alpha}(2)$$
(12.146)

in Rydbergs. Therefore

$$f(\alpha) = -2\alpha^{2} + \langle \psi_{100}^{\alpha}(1) | \frac{(\alpha - Z)e^{2}}{r_{1}} | \psi_{100}^{\alpha}(1) \rangle + \langle \psi_{100}^{\alpha}(2) | \frac{(\alpha - Z)e^{2}}{r_{2}} | \psi_{100}^{\alpha}(2) \rangle + \langle \psi(\alpha) | \frac{e^{2}}{r_{12}} | \psi(\alpha) \rangle$$
(12.147)

 But

$$\langle \psi_{100}^{\alpha}(1) | \frac{(\alpha - Z)e^2}{r_1} | \psi_{100}^{\alpha}(1) \rangle = \langle \psi_{100}^{\alpha}(2) | \frac{(\alpha - Z)e^2}{r_2} | \psi_{100}^{\alpha}(2) \rangle$$
$$= \langle 100 | \frac{(\alpha - Z)e^2}{r} | 100 \rangle$$
(12.148)

Therefore,

$$f(\alpha) = -2\alpha^2 + 2e^2(\alpha - Z) \langle 100| \frac{1}{r} |100\rangle + \langle 100| \langle 100| \frac{e^2}{r_{12}} |100\rangle |100\rangle \quad (12.149)$$

Using some earlier calculations we get

$$f(\alpha) = -2\alpha^2 + 4\alpha(\alpha - Z) + \frac{5}{4}\alpha$$
 (12.150)

Minimizing

$$\frac{df}{d\alpha} = 0 = -2\alpha + 2Z - \frac{5}{8}$$
(12.151)

 or

$$\alpha = Z - \frac{5}{16} \tag{12.152}$$

and

$$E_0^{\text{variational}} = f(Z - \frac{5}{16}) = -2(Z - \frac{5}{16})^2 = -2Z^2 + \frac{5}{4}Z - 2(\frac{5}{16})^2 \qquad (12.153)$$

The first two terms are just the first order perturbation theory result. The third term lowers the energy relative to perturbation theory.

For Z = 2, we get

$$\begin{split} E_0^{variational} &= -5.7 \; Ry = -77.48 \; eV \\ E_0^{experimental} &= -78.975 \; eV \\ E_0^{perturbation \; theory} &= -74.8 \; eV \end{split}$$

Even with the simple trial function, we get a significantly better result using the variational method. The reduction in the value of Z represents the effect of the inner electron screening the outer electron so it see a smaller nuclear charge.

12.6 Multielectron Atoms

We now return to the case of N electrons (N > 2). We have

$$\hat{H}\psi_{\alpha} = E_{\alpha}\psi_{\alpha} \tag{12.154}$$

where α = all quantum numbers needed to specify the N-electron state and the Hamiltonian \hat{H} is

$$\hat{H} = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m_e} \nabla_i^2 - \frac{Ze^2}{r_i} \right] + \sum_{i=1}^{N} \sum_{j>i}^{N} \frac{e^2}{r_{ij}}$$
(12.155)

For the moment we are neglecting many small(weak) interactions (spin-orbit, etc). We are also not including the electromagnetic field at this stage. We will consider it later when we talk about time-dependent perturbation theory and we will see that its presence leads to instability of atoms with respect to photon absorption/emission.

The electrons are all indistinguishable, which says that

$$\hat{H}, \hat{P}_{ij} = 0 \quad i, j = 1, 2, 3, \dots, N \; ; \; i \neq j$$

$$(12.156)$$

This implies, since electrons are fermions, that the wave functions must be completely antisymmetric, i.e.,

$$\hat{P}_{ij}\psi_{\alpha} = -\psi_{\alpha} \quad i, j = 1, 2, 3, \dots, N \; ; \; i \neq j$$

$$(12.157)$$

The full Hamiltonian is much too complex to solve exactly. We will approach the solution as a series of increasingly better approximations and obtain a qualitative picture of the energy level structure of these complex atoms.

Since the difficulties arise from the e^2/r_{ij} terms that represent the electronelectron repulsion, we start with a model where each electron moves independently of all the other electrons (an independent particle model). In this model each electron will be described by a single-particle wavefunction called an orbital.

This leads us to write an approximate Hamiltonian in terms of the single particle Hamiltonians

$$\hat{H}_{0i} = -\frac{\hbar^2}{2m_e} \nabla_i^2 - \hat{V}_i(\vec{r}_i)$$
(12.158)

where we assume that the potential energy of the i^{th} electron $\hat{V}_i(\vec{r}_i)$ does not depend on the coordinates of the other N-1 electrons. We then have the approximate Hamiltonian for the entire system

$$\hat{H}_{0}^{A} = \sum_{i=1}^{N} \hat{H}_{0i} = \sum_{i=1}^{N} \left[-\frac{\hbar^{2}}{2m_{e}} \nabla_{i}^{2} - \hat{V}_{i}(\vec{r}_{i}) \right]$$
(12.159)

This Hamiltonian is separable, i.e., we can assume that the system wavefunction is a product of single-particle wavefunctions or orbitals.

$$\psi_{\alpha} = \psi_{\varepsilon_1}(\vec{r}_1)\psi_{\varepsilon_2}(\vec{r}_2)\psi_{\varepsilon_3}(\vec{r}_3)\dots\psi_{\varepsilon_N}(\vec{r}_N)$$
(12.160)

where the subscript ε_k represents all applicable single particle quantum numbers for the k^{th} electron, that is,

$$\varepsilon_k = (n_i \ell_i m_{\ell_i} m_{s_i}) \tag{12.161}$$

Each single particle wave function is a product of the form

$$\psi_{\varepsilon} = (\text{spatial wave function})(\text{spin vector})$$
 (12.162)

We will assume that the system wavefunction is a completely antisymmetric combination of the product states ψ_{α} .

Each term in \hat{H}_0^A has an eigenvalue equation of the form

$$\left[-\frac{\hbar^2}{2m_e}\nabla_i^2 - \hat{V}_i(\vec{r}_i)\right]\psi_{n_i\ell_i m_{\ell_i} m_{s_i}} = E_{n_i\ell_i m_{\ell_i} m_{s_i}}\psi_{n_i\ell_i m_{\ell_i} m_{s_i}}$$
(12.163)

and there are N such equations.

To solve these equations, we must know the potential energy functions $\hat{V}_i(\vec{r}_i)$. As a first approximation within the orbital approximations, we ignore the electronelectron repulsion so that the electrons only interact with the nucleus and we have

$$\hat{V}_i(\vec{r}_i) = \hat{V}(r_i) = -\frac{Ze^2}{r_i}$$
(12.164)

In this approximation, all the other electrons do not matter at all and each electron satisfies

$$\left[-\frac{\hbar^2}{2m_e}\nabla_i^2 - \frac{Ze^2}{r_i}\right]\psi_{n_i\ell_i m_{\ell_i} m_{s_i}}(\vec{r}_i) = E_{n_i\ell_i m_{\ell_i} m_{s_i}}\psi_{n_i\ell_i m_{\ell_i} m_{s_i}}(\vec{r}_i) \qquad (12.165)$$

This is a hydrogen atom with charge Ze. The single-particle wavefunctions are given by

$$\psi_{n\ell m_{\ell}m_{s}}(\vec{r}) = R_{n\ell}(r)Y_{\ell m_{\ell}}(\theta,\varphi)\chi_{sm_{s}} = \psi_{\varepsilon}(\vec{r})$$
(12.166)

where

$$E_{n_k} \approx -\frac{m_e Z^2 e^4}{2\hbar^2 n_k} \qquad n_k = 1, 2, 3, \dots$$
 (12.167)

The wave function corresponding to a set of orbitals $(\varepsilon_1, \varepsilon_2, \dots, \varepsilon_N)$ is then properly antisymmetrized by writing it as

$$\psi_{\alpha} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{\varepsilon_{1}}(1) & \psi_{\varepsilon_{2}}(1) & \dots & \psi_{\varepsilon_{N}}(1) \\ \psi_{\varepsilon_{1}}(2) & \dots & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \psi_{\varepsilon_{1}}(N) & \dots & \dots & \psi_{\varepsilon_{N}}(N) \end{vmatrix}$$
(12.168)

where

$$E_{\alpha} = E_{\varepsilon_1} + E_{\varepsilon_2} + \dots + E_{\varepsilon_N} \tag{12.169}$$

We certainly can write down an answer in this approximation but the result, not surprisingly, is terrible. Any real electron is dramatically affected by the others, even when there is only one other electron as we saw in helium.

We move on by making the next incrementally better approximation. This involves the concept of screening.

12.6.1 Screening

Any electron, on the average, if it is far from the nucleus, does not feel all of the nuclear charge Ze and hence has a weaker Coulomb attraction then we have assumed. This is clear in the helium variational calculation where we found that the best value of the charge variational parameter Z' was

$$Z' = Z - \frac{5}{16} \tag{12.170}$$

This implies that, on the average, the distant electrons are *shielded* or *screened* from the nucleus by the other electrons.

What is the simplest correction that we can make to take this effect into account for multi-electron atoms and still leave us with solvable equations?

Suppose we write

$$V_i(r_i) = -\frac{Ze^2}{r_i} + V_i^{eff}(r_i)$$
(12.171)

where $V_i^{eff}(r_i)$ includes the screening effects of the other N-1 electrons. An important feature of this assumption is that $V_i^{eff}(r_i)$ is independent of (θ, φ) . This says that the angular part of the wave function is still

$$Y_{\ell_i m_{\ell_i}}(\theta, \varphi) \tag{12.172}$$

The radial function, however, now satisfies a modified equation

$$\frac{1}{r_i^2} \frac{d}{dr_i} \left[r_i^2 \frac{d}{dr_i} - \frac{\ell(\ell+1)}{r_i^2} + \frac{2m_e}{\hbar^2} \left(E_{n_i} - V_i(r_i) \right) \right] R_{n_i \ell_i}(r_i) = 0$$
(12.173)

This is called the *central field approximation*. We still have N difficult equations to solve.

Hartree proposed the following solution using a successive approximations technique.

- 1. an initial potential function is guessed (a very educated guess)
- 2. this potential function is used to derive new wave functions
- 3. the new wave functions generate a new potential energy function
- 4. the procedure is continued until the final wave functions determine a *self*-consistent potential, i.e., it stops changing as we iterate

The Hartree method is equivalent to a variational calculation, where the trial function is taken to be a simple product of single-particle orbitals and the variation is performed by varying each orbital in an arbitrary way.

Using single-particle wave functions, however, we are still neglecting the correlations between the electrons. Although the simple single-particle orbital product functions ignore antisymmetry, some effect of the Pauli exclusion principle (PEP) can be included in the calculations by choosing the single-particle quantum numbers so they do not violate the PEP.

If we make the calculation more complicated, we can include antisymmetry by using Slater determinant wave functions. This is called the Hartree-Fock theory. Correlation effects arising from the $1/r_{ij}$ terms can then be added using perturbation theory. At the level of this text, we assume that this can be done (see Bethe/Jackiw for details).

12.6.2 Shell Structure

The hydrogen atom solution exhibited a kind of shell structure. We found that the energy levels were given by

$$E_n = -\frac{Z^2 e^2}{2a_0 n^2} \tag{12.174}$$

and each level had a degeneracy equal to n^2 arising from the allowed ranges

$$\begin{split} \ell &= 0, 1, 2, \dots, n-1 \\ m_\ell &= -\ell, \dots, \ell \end{split}$$

We say that each n value defines a shell with energy E_n and within each shell we have subshells defined by ℓ . Thus,

$$\begin{split} n &= 1 \rightarrow \ell = 0 \rightarrow 1s \text{subshell} \\ n &= 2 \rightarrow \ell = 0, 1 \rightarrow 2s, 2p \text{subshells} \\ n &= 3 \rightarrow \ell = 0, 1, 2 \rightarrow 3s, 3p, 3d \text{subshells} \end{split}$$

We can generalize this idea to N electron atoms.

We assume that the atom consists of shells (n) and subshells $(n\ell)$. Electrons are placed into these shells so that we do not violate the PEP, that is, since the electrons are fermions only two electrons can be in each energy level. We define in this model

$$\langle r \rangle_{n0} = radius$$
 of a shell
 $\langle r \rangle_{n\ell} = radius$ of a subshell

and we have

$$E_{n\ell} = E_{n\ell'} \text{ (degenerate)} \tag{12.175}$$

(this is not true in the central field approximation).

For n > 1, the *s*-orbital has a nonzero probability near the origin r = 0 (the nucleus). This implies that it *penetrates* the n = 1 shell more than the corresponding *p*-orbitals do. This implies that the *s* subshell electrons feel a stronger nuclear charge then the *p* subshell electrons.

Therefore, we expect in this model that the energy levels will look like Figure 12.6 below.



Figure 12.6: Expected Level Structure

which is the *screening* effect.

Complex screening arguments of this type lead to the *Aufbau* principle, which tells us how electrons fill shells.

We see how it works by figuring out the ground state of an N electron atom. The ground state corresponds to that state where all the *lowest energy levels* are filled with a *maximum* of two electrons per level. It is clear that this is the state of lowest energy.

The single-particle Hamiltonian in the central field approximation commutes with ℓ_{iz} and s_{iz} which implies that the energy levels are independent of m_{ℓ_i} and m_{s_i} . Each energy level is therefore characterized by the 2N quantum numbers

$$n_i, \ell_i \quad i = 1, 2, 3, \dots, N$$
 (12.176)

We define the electronic configuration of an atomic state as the set of quantum numbers (n_i, ℓ_i) for all the electrons in the atom. We use the symbolic representation

$$shell - label = (n - label)(\ell - label)^{number of electrons}$$
(12.177)

i.e.,

ground state of hydrogen =
$$1s^{1} = 1s$$

(a superscript 1 is always understood)
ground state of helium = $1s^{2}$
ground state of lithium = $1s^{2}2s$

The electronic configuration of helium is an example of a *closed* or *full* shell. The 1s subshell has the maximum number electrons as allowed by the PEP, i.e.,

$$n = 1, \ell = 0, m_{\ell} = 0, s = \frac{1}{2}, m_s = \pm \frac{1}{2}$$
(12.178)

The Aufbau principle says that we fill the shells so that we obey the PEP or in the order

$$1s, 2s, 2p, 3s, 3p, 3d, 4s, \dots$$

with energy increasing from left to right.

The screening arguments of the type we just discussed imply that for a given n (a given shell) the energy order is s, p, d, \ldots and generally the energy of a shell increases with n = the principal quantum number. The closed shells correspond to

$$s - shell \rightarrow \text{maximum number of electrons} = 2$$

= 2(2 ℓ + 1)
 $p - shell \rightarrow \text{maximum number of electrons} = 6$
 $d - shell \rightarrow \text{maximum number of electrons} = 10$

and so on.

Electrons in the shell beyond the last closed shell are called *valence* electrons.

Much of the form and shape of the periodic table is determined by the Aufbau principle. For instance

number of valence electrons \rightarrow chemical properties

The valence electrons are the ones that participate in bonding and chemical reactions.

This implies that

$$carbon \rightarrow 1s^2 2s^2 2p^2$$

and
 $silicon \rightarrow 1s^2 2s^2 2p^6 3s^2 3p^2$

which each have two p valence electrons should have similar chemical properties, which is the case.

As with all simple principles of this type, anomalies and breakdowns soon appear. For the Aufbau principle this occurs at the n = 3 shell.

In real atoms, when the 3d and 4s subshells are partially full, the 4s level fills ups before the 3d level. This means that

$$potassium \rightarrow 1s^2 2s^2 2p^2 3s^2 3p^6 4s$$

and not $1s^2 2s^2 2p^6 3s^2 3p^6 3d$

The 4s state has a larger probability of being near r = 0 then the 3d state and hence its energy is lower.

For neutral atoms, an experimental ordering scheme is



At the level of this text we will not be doing any actual energy calculations.

12.7 Angular Momentum Coupling

The N electrons each have spin and orbital angular momentum and thus have associated magnetic moments.

For the full Hamiltonian \hat{H} including the electron-electron repulsion terms we have

$$\left[\hat{H}, \vec{\ell}_{i,op}\right] \neq 0 \quad i = 1, 2, 3, \dots, N$$
 (12.179)

However,

$$\left[\hat{H}, \vec{L}_{op}\right] = 0 \tag{12.180}$$

where

$$\vec{L}_{op} = \sum_{i=1}^{N} \vec{\ell}_{i,op}$$
 = the total orbital angular momentum (12.181)

Therefore, the individual ℓ_i are not conserved, but \vec{L} is conserved.

Thus, the electron-electron repulsion or electrostatic terms in the Hamiltonian couple the electron orbital angular momenta.

In addition, we must add in spin-orbit and other magnetic interactions (spinspin, etc).

The spin-orbit interaction leads to terms of the form $\vec{\ell}_i \cdot \vec{s}_i$ and thus couple a particle's orbital and spin angular momentum leading to (j_i, m_{j_i}) values, where $\vec{j}_i = \vec{\ell}_i + \vec{s}_i$ as we saw earlier in hydrogen.

In most light atoms, the magnetic interactions are usually weaker than the electrostatic interactions, i.e., electrostatic $\approx 1 \ eV$ and spin-orbit $\approx 10^{-4} - 10^{-5} \ eV$.

The angular momentum coupling in a light atom goes like:

1. the orbital angular momenta $\vec{\ell}_i$ couple to form a total orbital angular momentum

$$\vec{L}_{op} = \sum_{i=1}^{N} \vec{\ell}_{i,op}$$
(12.182)

2. the spin angular momenta \vec{s}_i couple to form a total spin angular momentum

$$\vec{S}_{op} = \sum_{i=1}^{N} \vec{s}_{i,op}$$
 (12.183)

These two couplings occur when we include the electrostatic interactions in the Hamiltonian \hat{H} .

3. the weaker magnetic interactions then couple \vec{L} and \vec{S} to form the total angular momentum of the atom

$$\vec{J} = \vec{L} + \vec{S} \tag{12.184}$$

This coupling scheme or order where the electrostatic interactions dominate the magnetic interactions is called LS or *Russell-Saunders* coupling.

In heavy atoms, the spin-orbit magnetic interactions dominate the electrostatic interactions and we get an alternative coupling scheme:

1. each electron's $\vec{\ell}_i$ and \vec{s}_i couple via the magnetic interactions to form

$$\vec{j}_i = \vec{\ell}_i + \vec{s}_i$$

= the total angular momentum for the i^{th} electron

2. the electrostatic interactions then couple the \vec{j}_i to form

$$\vec{J}_{op} = \sum_{i=1}^{N} \vec{j}_{i,op}$$
(12.185)

This scheme is called *jj-coupling*.

We will now investigate the energy level structure in detail for these two different schemes.

Our discussion of helium has shown that exchange symmetry, which requires that the wave functions are completely antisymmetric, has dramatic observable consequences. We saw a spin-spin correlation energy that is characterized by the rule:

There is a tendency for electrons with parallel spins to repel (avoid) each other. This fact, together with the electrostatic repulsion between electrons implies a strong exchange correlation that cause the spins to tend to align with each other

12.7.1 LS Coupling

In this regime we have the observables and quantum numbers as shown in Table 12.3 below:

| Operator | Quantum Number |
|------------------|----------------|
| \vec{L}_{op}^2 | L |
| $\vec{J_{op}^2}$ | J |
| \vec{S}_{op}^2 | S |
| \hat{L}_z | M_L |
| \hat{S}_z | M_S |

Table 12.3: LS Coupling Quantum Numbers

When we discussed the spin-orbit interaction in hydrogen we found

- 1. when we neglect \hat{H}_{so} we can use either $|n,L,S,M_L,M_S\rangle$ or $|n,L,S,J,M_J\rangle$ as basis states
- 2. when we add in \hat{H}_{so} , M_L and M_S are no longer conserved (not good quantum numbers) and therefore we must use $|n, L, S, J, M_J\rangle$ as basis states

Now in the orbital approximation we have

$$M_L = \sum_{i=1}^{N} m_{\ell_i} \quad , \quad M_S = \sum_{i=1}^{N} m_{s_i} \tag{12.186}$$

and

$$\hat{L}_z \psi_\alpha = \hbar M_L \psi_\alpha \qquad \hat{S}_z \psi_\alpha = \hbar M_S \psi_\alpha$$

What are the possible L,S values? We can use our addition of angular momentum rules to find out.

Consider two p-electrons , i.e., an vp^2 configuration. We have

$$\ell_1 = \ell_2 = 1 \to L = 0, 1, 2$$
$$s_1 = s_2 = \frac{1}{2} \to S = 0, 1$$

and

for a given
$$L$$
 $M_L = -L, \dots, L$
for a given S $M_S = -S, \dots, S$

and

$$M_J = M_L + M_S$$
$$J = |L - S|, \dots, L + S$$

Therefore we get the possibilities shown in Table 12.4 below:

| L | S | J | State(s) |
|---|---|-------------|-------------------|
| 0 | 0 | 0 | $^{1}S_{0}$ |
| 0 | 1 | 1 | ${}^{3}S_{1}$ |
| 1 | 0 | 1 | ${}^{1}P_{1}$ |
| 1 | 1 | $0,\!1,\!2$ | ${}^{3}P_{0,1,2}$ |
| 2 | 0 | 2 | ${}^{1}D_{1}$ |
| 2 | 1 | 1,2,3 | $^{3}D_{1,2,3}$ |

Table 12.4: Possible States

We will discuss the state notation shortly.

For a closed shell we must have L = S = 0 or we would violate the PEP. For example,

$$s^2 \rightarrow \ell_1 = \ell_2 = 0 \rightarrow L = 0$$
$$s_1 = s_2 = \frac{1}{2} \rightarrow S = 0 \text{ or } 1$$

However, there is only one way to choose the m quantum numbers without violating the PEP which is shown in Table 12.5 below.

| m_{ℓ_1} | m_{ℓ_2} | m_{s_1} | m_{s_2} |
|--------------|--------------|-----------|-----------|
| 0 | 0 | 1/2 | -1/2 |

Table 12.5: s^2 m-values

We therefore have M_L = M_S = 0 (only possibility) which implies that

$$L = S = J = 0 \to {}^{1}S_{0}$$
 state (12.187)

For

$$p^{6} \rightarrow \ell_{1} = \ell_{2} = \ell_{3} = \ell_{4} = \ell_{5} = \ell_{6} = 1$$
$$s_{1} = s_{2} = s_{3} = s_{4} = s_{5} = s_{6} = \frac{1}{2}$$

Once again it turns out there is only one way to choose the values without violating the PEP. This is shown in Table 12.6 below.

| m_{ℓ_1} | m_{ℓ_2} | m_{ℓ_3} | m_{ℓ_4} | m_{ℓ_5} | m_{ℓ_6} | m_{s_1} | m_{s_2} | m_{s_3} | m_{s_4} | m_{s_5} | m_{s_6} |
|--------------|--------------|--------------|--------------|--------------|--------------|-----------|-----------|-----------|-----------|-----------|-----------|
| 1 | 1 | 0 | 0 | -1 | -1 | 1/2 | -1/2 | 1/2 | -1/2 | 1/2 | -1/2 |

Table 12.6: p^6 m-values

We therefore have $M_L = M_S = 0$ (only possibility) which implies that

$$L = S = J = 0 \to {}^{1}S_{0} \text{ state}$$
 (12.188)

This result is true for *all* closed shells.

In the presence of \hat{H}_{so} the energy levels will depend on L, S and J but not on M_L, M_S or M_J , which is why we label their *atomic terms* by

$$^{2S+1}L_J$$
 (12.189)

where

$$S, P, D, F, \dots$$
 means $L = 0, 1, 2, 3, \dots$ (12.190)

The superscript 2S + 1 s the *multiplicity* of the level (singlet, doublet, triplet, etc).

If we ignore \hat{H}_{so} then we have (2S+1)(2L+1) degeneracy for a given level.

Adding \hat{H}_{so} splits the J states. Each term ${}^{2S+1}L_J$ remains 2J + 1 degenerate (the M_J values).

This degeneracy is removed by an external magnetic field which splits the 2J+1 M_J levels(Zeeman effect).

How do we determine the ground state for a particular atom in this scheme?

First, we fill up as many closed shells as possible. The remaining (valence) electrons determine the ground state configuration.

Let us consider carbon which has two equivalent (same subshell) 2p-electrons in the unfilled shell. We have

$$2p^2 \rightarrow \ell_1 = \ell_2 = 1 \rightarrow L = 0, 1 \text{ or } 2$$
$$s_1 = s_2 = \frac{1}{2} \rightarrow S = 0 \text{ or } 1$$

We get Table 12.7 below by applying these rules:

| L | S | J | Term | Sublevels |
|---|---|-------------|---------|-----------------|
| 0 | 0 | 0 | ^{1}S | ${}^{1}S_{0}$ |
| 1 | 0 | 1 | ^{1}P | ${}^{1}P_{1}$ |
| 2 | 0 | 2 | ^{1}D | $^{1}D_{2}$ |
| 0 | 1 | 1 | ^{3}S | ${}^{3}S_{1}$ |
| 1 | 1 | $0,\!1,\!2$ | ^{3}P | $^{3}P_{0,1,2}$ |
| 2 | 1 | 1,2,3 | ^{3}D | $^{3}D_{1,2,3}$ |

Table 12.7: Possible States from LS Rules

Not all of these sublevels are allowed by the PEP however. To see this we must look at the individual electron quantum numbers. Table 12.8 below shows those $m_{\ell_1}, m_{\ell_2}, m_{s_1}, m_{s_2}$ values allowed by the PEP (i.e., no two electrons have the same set of quantum numbers).

Before proceeding to the table, in this case, we can use symmetry arguments to determine the allowed levels. In the special case of only two electrons in an unfilled shell, we can easily determine the symmetry of the spin vectors

> $S = 0 \rightarrow$ antisymmetric spin function $S = 1 \rightarrow$ symmetric spin function

We also know the symmetry of the spatial state in general. The symmetry follows from the symmetry of the angular part of the 2-electron wave function. Since we have a central field approximation, the angular part of the wave function is given by the Y_{LM_L} spherical harmonics. The radial function is always symmetric. The symmetry of the spherical harmonics is $(-1)^L$. Therefore,

> $L = odd \rightarrow$ antisymmetric space function $L = even \rightarrow$ symmetric space function

The product of the spin vector and the spatial function must always be antisymmetric. Therefore we have

> S = 0 always combines with even LS = 1 always combines with odd L

This method is only simple to carry out for 2–electron unfilled shells. In the case of carbon we get the allowed states

$$L = 2, S = 0 \rightarrow 5 \text{ states } = (2L+1)(2S+1)$$
$$L = 1, S = 1 \rightarrow 9 \text{ states}$$
$$L = 0, S = 0 \rightarrow 1 \text{ states}$$

for a total of 15 allowed states. The individual quantum numbers table corresponding to these 15 states is

| Entry | m_ℓ = -1 | m_ℓ = 0 | m_ℓ = +1 | M_L | M_S |
|-------|---------------|--------------|---------------|-------|-------|
| 1 | ↑↓ | | | -2 | 0 |
| 2 | | ↑↓ | | 0 | 0 |
| 3 | | | ^↓ | 2 | 0 |
| 4 | 1 | 1 | | -1 | 1 |
| 5 | 1 | \downarrow | | -1 | 0 |
| 6 | \downarrow | 1 | | -1 | 0 |
| 7 | \downarrow | \downarrow | | -1 | -1 |
| 8 | 1 | | 1 | 0 | 1 |
| 9 | 1 | | \downarrow | 0 | 0 |
| 10 | Ļ | | 1 | 0 | 0 |
| 11 | \downarrow | | \downarrow | 0 | -1 |
| 12 | | 1 | 1 | 1 | 1 |
| 13 | | 1 | \downarrow | 1 | 0 |
| 14 | | \downarrow | 1 | 1 | 0 |
| 15 | | \downarrow | \downarrow | 1 | -1 |

Table 12.8: Individual Quantum Numbers

Any other combinations will violate the PEP. This table can be constructed just using the PEP.

We now construct an implied terms table which tells us how many states exist with a particular pair of (M_L, M_S) values. It is shown as Table 12.9 below.

| M_L/M_S | 1 | 0 | -1 |
|-----------|---|---|----|
| 2 | 0 | 1 | 0 |
| 1 | 1 | 2 | 1 |
| 0 | 1 | 3 | 1 |
| -1 | 1 | 2 | 1 |
| -2 | 0 | 1 | 0 |

Table 12.9: Implied terms

We use this table to determine which atomic terms are allowed for carbon. The steps are as follows:

1. Consider the largest possible values of L and S, L = 2,S = 1 which correspond to the ${}^{3}D$ terms.

Now if a ${}^{3}D$ atomic term existed , then we would necessarily have $M_{L} = 2, M_{S} = 1$ terms. However, there are no such terms, which implies that the ${}^{3}D$ term is not allowed and thus the sublevels ${}^{3}D_{1}, {}^{3}D_{2}, {}^{3}D_{3}$ are ruled out

by the PEP.

- 2. We now look at the next largest values, namely, L = 2, S = 0 or the ${}^{1}D$ term. A L = 2, S = 0 term requires $M_{L} = 2, M_{S} = 0$ terms which do exist. Therefore the ${}^{1}D$ term and the sublevel ${}^{1}D_{2}$ exist. This has J = 2 and thus $2J + 1 = 5 M_{J}$ levels. This accounts for 5 of the 15 entries in the table.
- 3. We subtract these 5 states to get a second-implied terms table

| M_L/M_S | 1 | 0 | -1 |
|-----------|---|---|----|
| 2 | 0 | 0 | 0 |
| 1 | 1 | 1 | 1 |
| 0 | 1 | 2 | 1 |
| -1 | 1 | 1 | 1 |
| -2 | 0 | 0 | 0 |

Table 12.10: Implied terms

- 4. We now look at the next largest values, namely, L = 1, S = 1 or the ${}^{3}P$ term. Since entries with $M_{L} = -1, 0, +1$ and $M_{S} = -1, 0, +1$ still exist in the new table, the ${}^{3}P$ term and the sublevels ${}^{3}P_{2}, {}^{3}P_{1}, {}^{3}P_{0}$ are allowed. These correspond to a total of (2L + 1)(2S + 1) = 5 + 3 + 1 = 9 states.
- 5. We subtract these 9 states to get the third-implied terms table

| M_L/M_S | 1 | 0 | -1 |
|-----------|---|---|----|
| 2 | 0 | 0 | 0 |
| 1 | 0 | 0 | 0 |
| 0 | 0 | 1 | 0 |
| -1 | 0 | 0 | 0 |
| -2 | 0 | 0 | 0 |

Table 12.11: Implied terms

Only one state is left with $M_L = M_S = 0$, which is a ¹S atomic term. Therefore the ¹S₀ sublevel is allowed.

This accounts for all the 15 entries in the table. No more states are allowed, which means that the ${}^{3}S$ and ${}^{1}P$ atomic terms and their associated sublevels are forbidden by the PEP. This result agrees with the allowed states we obtained from symmetry arguments.

We always need to use the implied-terms tables in the general cases (more than

2 electrons in an unfilled shell) because the corresponding symmetry arguments are very complex to apply.

Finally, for carbon we have the ${}^{1}S$, ${}^{3}P$ and ${}^{1}D$ allowed by the PEP.

This result is true for all atoms with 2 equivalent p-electrons outside closed subshells.

To complete the picture, we must now determine how the allowed terms are ordered in energy.

12.7.2 Hund's Rules

Each sublevel in carbon ${}^{1}S_{0}$, ${}^{3}P_{2}$, ${}^{3}P_{1}$, ${}^{3}P_{0}$ and ${}^{1}D_{2}$ has a different energy when \hat{H}_{so} is included in \hat{H} .

A set of rules exists for qualitatively ordering the levels. They are called Hund's rules.

Hund's rules apply when we are ordering the energy levels and sublevels for equivalent electrons in the ground state.

Rule 1 Terms in the ground state configuration with maximum multiplicity 2S + 1 lie lowest in energy.

This follows from the fact that same spins (unpaired spins) *repel* and different spins (paired spins) *attract*.

High multiplicity implies a greater number of electrons with parallel spin than low multiplicity in multielectron atoms. Since parallel spin electrons avoid each other, the e^2/r_{ij} effect decreases and the energy of high multiplicity states lies below that of low multiplicity states.

Rule 2 Of several levels with the same multiplicity S, the one with maximum L lies lowest in energy

In some sense, the maximum L state implies that all electrons are *orbiting in* the same direction. These electrons tend to remain separated from each other and so have a lower energy than those orbiting in the opposite direction, which get close to each other some of the time.

Rule 2 Of several sublevels with the same multiplicity S and same L

- 1. the sublevel with the minimum value of J lies lowest in energy if the shell is less than half-filled. These are called *regular multiplets*
- 2. the sublevel with the maximum value of J lies lowest in energy if the shell

is more than half-filled. These are called *inverted multiplets*

This results follows from \hat{H}_{so} and the fact that $-e^2/r$ increases as $r \to \infty$. Applying Hund's rules to an np^2 configuration we get the energy level scheme in Figure 12.7 below.



Figure 12.7: np^2 Level Scheme

Hund's rules are not perfect since they are based on the orbital approximation.

To determine an electronic configuration, we must specify how the electrons are placed into subshells. It turns out there is a phenomenon called configuration interaction or configuration mixing which forces the quantum mechanical state to sometimes be a mixture of more than one configuration.

12.7.3 JJ-Coupling

In heavy atoms, the magnetic interactions which couple the \vec{l}_i and \vec{s}_i together into the \vec{j}_i , dominate over the electrostatic interactions which led to LS coupling. The configurations are then better described by the so-called *jj-coupling* scheme.

Since $s_i = 1/2$ for all electrons, we have for $\ell_i \ge 1$

$$j_i = \ell_i \pm \frac{1}{2}$$
$$m_{j_i} = -j_i, \dots, j_i$$

The individual \vec{j}_i then couple together to give the total \vec{J} .

In a two-electron configuration the levels are labelled by J, j_1, j_2, M_J where

$$J = |j_1 - j_2|, \dots, j_1 + j_2$$
$$M_J = -J, \dots, J$$

Let us consider the Pb (lead) atom, which has np^2 valence electrons (built on many closed shells). We have

$$\ell_1 = \ell_2 = 1$$

 $\rightarrow j_1 = \frac{1}{2}, \frac{3}{2} \text{ and } j_2 = \frac{1}{2}, \frac{3}{2}$

The possible total J values are then

$$\frac{3}{2} \otimes \frac{3}{2} = 3, 2, 1, 0$$
$$\frac{1}{2} \otimes \frac{3}{2} = 2, 1$$
$$\frac{1}{2} \otimes \frac{1}{2} = 1, 0$$

Not all of these states are allowed by the PEP. For example,

$$J = 3, M_J = 3 \rightarrow j_1 = j_2 = \frac{3}{2}, m_{j1} = m_{j2} = \frac{3}{2}$$
$$\ell_1 = \ell_2 = 1, m_{\ell 1} = m_{\ell 2} = 1$$
$$s_1 = s_2 = \frac{1}{2}, m_{s1} = m_{s2} = \frac{1}{2}$$

Both electrons need to have identical quantum numbers for this state to exist. Thus, this state is not allowed. In a similar manner,

$$J = 3$$
 , $j_1 = j_2 = \frac{3}{2}$
 $J = 1$, $j_1 = j_2 = \frac{1}{2}$

can be shown to be forbidden by the PEP. Therefore we have

$$\frac{3}{2} \otimes \frac{3}{2} = 2,0$$
$$\frac{1}{2} \otimes \frac{3}{2} = 2,1$$
$$\frac{1}{2} \otimes \frac{1}{2} = 0$$

Usually, the level with the lowest J for a given pair (j_1, j_2) has the lowest energy (this is not a strict rule).

For medium weight atoms, neither LS nor jj coupling is valid.

There is a connection between the levels in the two schemes as illustrated by the energy level diagram in Figure 12.8 below.



Figure 12.8: LS - jj Energy Level Connection

The connection between the two schemes is clear.

The spacing between J-levels in LS coupling is given as follows.

$$\langle \hat{H}_{so} \rangle = \frac{1}{2} C \left[(J(J+1) - L(L+1) - S(S+1)) \right]$$
 (12.191)

For the same L, S we have

$$E_{J+1} - E_J = \frac{1}{2}C\left[(J+1)(J+2) - J(J+1)\right]$$

= C(J+1) (12.192)

This says that the spacing between consecutive levels of a fine structure multiplet is proportional to the larger J value involved. This is the *Lande interval rule*.

We end this discussion with an example of two electrons that are not equivalent(in different shells). The discussion is more straightforward since we do not have to worry about the PEP (all possibilities are allowed).

We consider two electrons in a 4p4d configuration. In the LS coupling scheme

we have:

$$\begin{split} \ell_1 &= 1 \ , \ \ell_2 = 2 \rightarrow L = 1, 2, 3 \\ s_1 &= s_2 = \frac{1}{2} \rightarrow S = 0, 1 \\ 3 \otimes 1 \rightarrow J = 4, 3, 2 \\ 3 \otimes 0 \rightarrow J = 3 \rightarrow 7 \ \text{states} \\ 2 \otimes 1 \rightarrow J = 3, 2, 1 \rightarrow 16 \ \text{states} \\ 2 \otimes 0 \rightarrow J = 2 \rightarrow 5 \ \text{states} \\ 1 \otimes 1 \rightarrow J = 2, 1, 0 \rightarrow 9 \ \text{states} \\ 1 \otimes 0 \rightarrow J = 1 \rightarrow 3 \ \text{states} \end{split}$$

or

| J = 4 | in | 1 | level |
|-------|----|---|--------|
| J = 3 | in | 3 | levels |
| J = 2 | in | 4 | levels |
| J = 1 | in | 3 | levels |
| J = 0 | in | 1 | level |

Thus, we have 12 total levels. The LS coupling energy level diagram is shown in Figure 12.9 $\,$



Figure 12.9: LS 4p4d Energy Levels

In the jj-coupling scheme the energy leveldiagram is shown in Figure 12.10



Figure 12.10: jj 4p4d Energy Levels

Notice that the final J values are identical, but their arrangement in energy is very different.

12.8 Spherical Harmonics Addition Theorem

In Chapter 9 we defined the properties of the spherical harmonics. We found the following results.

12.8.1 Orbital Angular Momentum

Abstractly,

$$\left[\hat{L}_{i},\hat{L}_{j}\right] = i\hbar\varepsilon_{ijk}\hat{L}_{k} \text{ and } \left[\hat{L}_{on}^{2},\hat{L}_{j}\right] = 0$$
(12.193)

$$\hat{L}_{an}^{2}|\ell m\rangle = \hbar^{2}\ell(\ell+1)|\ell m\rangle \text{ and } \hat{L}_{3}|\ell m\rangle = \hbar m |\ell m\rangle$$
(12.194)

$$\hat{L}_{+} = \hat{L}_{x} \pm i\hat{L}_{y} \tag{12.195}$$

$$\ell = \frac{\text{integer}}{2} \ge 0 \tag{12.196}$$

For a given value of ℓ , m takes on the $2\ell + 1$ values

$$m = -\ell, -\ell + 1, -\ell + 2, \dots, \ell - 2, \ell - 1, \ell$$
In ordinary 3–dimensional space, if we define

$$Y_{\ell m}(\theta,\varphi) = \langle \theta\varphi \mid \ell m \rangle = spherical harmonic$$
(12.197)

then we have the defining equations for the $Y_{\ell m}(\theta, \varphi)$ given by

$$\langle \theta \varphi | \vec{L}_{op}^2 | \ell m \rangle = \vec{L}_{op}^2 \langle \theta \varphi | \ell m \rangle = \vec{L}_{op}^2 Y_{\ell m}(\theta, \varphi)$$

= $\hbar^2 \ell (\ell + 1) \langle \theta \varphi | \ell m \rangle = \hbar^2 \ell (\ell + 1) Y_{\ell m}(\theta, \varphi)$ (12.198)

$$\langle \theta \varphi | L_3 | \ell m \rangle = L_3 \langle \theta \varphi | \ell m \rangle = L_3 Y_{\ell m}(\theta, \varphi)$$

= $\hbar m \langle \theta \varphi | \ell m \rangle = \hbar m Y_{\ell m}(\theta, \varphi)$ (12.199)

The general result is

$$Y_{\ell m}(\theta,\varphi) - \frac{(-1)\ell}{2^{\ell}\ell!} \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell+m)!}{(\ell-m)!}} \frac{e^{im\varphi}}{(\sin\theta)^m} \left(\frac{d}{d\cos\theta}\right)^{\ell-m} (\sin\theta)^{2\ell} \quad (12.200)$$

Some examples are:

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$
(12.201)

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta , \ Y_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} e^{\pm i\varphi} \sin\theta$$
(12.202)

$$Y_{20} = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1) , \ Y_{2,\pm 1} = \mp \sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta e^{\pm i\varphi}$$
(12.203)

$$Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\varphi}$$
(12.204)

Some Properties

Complex Conjugate

$$Y_{\ell,-m}(\theta,\varphi) = (-1)^m Y^*_{\ell,m}(\theta,\varphi)$$
(12.205)

Under the parity operation

 $\vec{r} \rightarrow -\vec{r}$ or $r \rightarrow r, \theta \rightarrow \pi - \theta, \varphi \rightarrow \varphi + \pi$

which says that

$$e^{im\varphi} \to e^{im\varphi}e^{im\pi} = (-1)^m e^{im\varphi}$$
$$\sin\theta \to \sin(\pi - \theta) \to \sin\theta$$
$$\cos\theta \to \cos(\pi - \theta) \to -\cos\theta$$

which imply that

$$Y_{\ell,m}(\theta,\varphi) \to (-1)^{\ell} Y_{\ell,m}(\theta,\varphi)$$
(12.206)

Therefore,

if ℓ is even, then we have an even parity state if ℓ is odd, then we have an odd parity state

Since they form a complete set, any function of (θ, φ) can be expanded in terms of the $Y_{\ell,m}(\theta, \varphi)$ (the $Y_{\ell,m}(\theta, \varphi)$ are a basis), i.e., we can write

$$f(\theta,\varphi) = \sum_{\ell,m} f_{\ell m} Y_{\ell,m}(\theta,\varphi)$$
(12.207)

where

$$f_{\ell m} = \int_{0}^{2\pi} d\varphi \int_{0}^{\pi} \sin \theta d\theta Y^*_{\ell' m'}(\theta, \varphi) f(\theta, \varphi)$$
(12.208)

and we have used the orthonormality relation

$$\int_{0}^{2\pi} d\varphi \int_{0}^{\pi} \sin\theta d\theta Y_{\ell'm'}^{*}(\theta,\varphi) Y_{\ell m}(\theta,\varphi) = \delta_{\ell'\ell} \delta_{m'm}$$
(12.209)

The spherical harmonics also satisfy these relations:

Closure:

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_{\ell m}^{*}(\theta,\phi) Y_{\ell m}(\theta',\phi') = \frac{\delta(\theta-\theta')\delta(\phi-\phi')}{\sin\theta} \equiv \delta(\hat{r},\hat{r}')$$
(12.210)

i.e., the solid angle delta function is equal to zero unless the two vectors $\hat{r}(\theta, \phi)$, $\hat{r}'(\theta', \phi')$ coincide. It has the property

$$\int f(\hat{r}')\delta(\hat{r},\hat{r}')d\Omega' = f(\hat{r})$$
(12.211)

for any function $f(\vec{r})$ of the spatial direction specified by θ, φ .

Recursion:

$$\hat{L}_{\pm}Y_{\ell m} = \left[\ell(\ell+1) - m(m\pm1)\right]^{1/2} Y_{\ell,m\pm1}$$

$$= \left[(\ell \mp m)(\ell+1\pm m)\right]^{1/2} Y_{\ell,m\pm1} \qquad (12.212)$$

$$\cos\theta Y_{\ell m} = \left[\frac{(\ell+1+m)(\ell+1-m)}{(2\ell+1)(2\ell+3)}\right]^{1/2} Y_{\ell+1,m}$$

$$+ \left[\frac{(\ell+m)(\ell-m)}{(2\ell+1)(2\ell-1)}\right]^{1/2} Y_{\ell-1,m} \qquad (12.213)$$



Figure 12.11: Angles Used in the Addition Theorem

12.8.2 The Addition Theorem

Consider two coordinate systems xyz and x'y'z'. The addition theorem is the formula expressing the eigenfunction $P_{\ell}(\cos \theta')$ of the angular momentum $\hat{L}_{z'}$ about the z'-axis in terms of the eigenfunctions $Y_{\ell,m}(\theta,\varphi)$ of \hat{L}_z . See Figure 12.11 below for orientations.

The angles α and β are the azimuth and the polar angles of the z' axis in the Cartesian xyz coordinate frame. They are also the first two Euler angles specifying the orientation of the Cartesian coordinate system x'y'z' with respect to xyz. The third Euler angle γ is left unspecified here and the x' and y' axes are not shown. The projections of the z' axis and the radius vector on the xy plane are dashed lines.

As we can see the position vector \vec{r} has angular coordinates θ, φ and θ', φ' in the two coordinate systems.

The direction of the z' axis in space is specified by its polar angle β and its azimuth angle α with respect to the xyz system.

Since P_{ℓ} is an eigenfunction of \vec{L}_{op}^2 , only spherical harmonics with the same subscript ℓ can appear in the expansion.

An interchange of θ , φ and β , α is equivalent to the transformation $\theta \to -\theta'$ and must leave the expansion unchanged because $P_{\ell}(\cos \theta')$ is an even function of θ' . This means that $P_{\ell}(\cos \theta')$ must be a function of $\varphi - \alpha$.

All of these requirements are satisfied only if we write

$$P_{\ell}(\cos\theta') = \sum_{m=-\ell}^{\ell} c_m Y_{\ell,-m}(\beta,\alpha) Y_{\ell,m}(\theta,\phi)$$
(12.214)

We determine the coefficients c_m using the conditions

$$\hat{L}_{z'} P_{\ell}(\cos \theta') = 0 \tag{12.215}$$

We also use the identity (from rotation of a vector component)

$$\hat{L}_{z'} = \sin\beta\cos\alpha\hat{L}_x + \sin\beta\sin\alpha\hat{L}_y + \cos\beta\hat{L}_z$$
$$= \frac{1}{2}\sin\beta e^{-i\alpha}\hat{L}_+ + \frac{1}{2}\sin\beta e^{i\alpha}\hat{L}_- + \cos\beta\hat{L}_z$$
(12.216)

and invoke the linear independence of the spherical harmonics to obtain (after some algebra)

$$c_{m\pm 1} = -c_m \to c_m = (-1)^m c_0 \tag{12.217}$$

so that we only need to determine c_0 . We specialize to $\beta = 0$ or $\theta' = \theta$ so that we have the relations

$$Y_{\ell m}(0,\phi) = \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m0}$$
(12.218)

$$Y_{\ell 0}(\theta, \phi) = \sqrt{\frac{2\ell + 1}{4\pi}} P_{\ell}(\cos \theta)$$
 (12.219)

We then have

$$P_{\ell}(\cos\theta) = \sum_{m=-\ell}^{\ell} c_m Y_{\ell,-m}(0,\alpha) Y_{\ell,m}(\theta,\phi) = \sum_{m=-\ell}^{\ell} c_m \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m0} Y_{\ell,m}(\theta,\phi)$$
$$= c_0 \sqrt{\frac{2\ell+1}{4\pi}} Y_{\ell,0}(\theta,\phi) = c_0 \sqrt{\frac{2\ell+1}{4\pi}} \sqrt{\frac{2\ell+1}{4\pi}} P_{\ell}(\cos\theta) \qquad (12.220)$$

or

$$c_0 = \frac{4\pi}{2\ell + 1} \tag{12.221}$$

and we end up with the addition theorem

$$P_{\ell}(\cos\theta') = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} c_m Y_{\ell m}^*(\beta,\alpha) Y_{\ell,m}(\theta,\phi)$$
(12.222)

where θ' = angle between the directions (β, α) and (θ, φ) .

If we combine the closure relation with the addition theorem we get the identity

$$\sum_{\ell=0}^{\infty} (2\ell+1) P_{\ell}(\hat{r} \cdot \hat{r}') = 4\pi \delta(\hat{r}, \hat{r}')$$
(12.223)

Since we can write

$$\delta(\vec{r} - \vec{r}') = \frac{\delta(r - r')}{r^2} \delta(\hat{r}, \hat{r}') \qquad (12.224)$$

we then have the identity

$$\delta(\vec{r} - \vec{r}') = \frac{\delta(r - r')}{r^2} \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{4\pi} P_{\ell}(\hat{r} \cdot \hat{r}')$$
(12.225)

Another useful relation is

$$e^{ikz} = \sum_{\ell=0}^{\infty} (2\ell+1)i^{\ell} j_{\ell}(kr) P_{\ell}(\cos\theta)$$
 (12.226)

or, in general

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^{\ell} j_{\ell}(kr) Y_{\ell m}^{*}(\theta_{\vec{k}}, \phi_{\vec{k}}) Y_{\ell m}(\theta_{\vec{r}}, \phi_{\vec{r}})$$
(12.227)

12.9 Problems

12.9.1 Two Bosons in a Well

Two identical spin-zero bosons are placed in a 1–dimensional square potential well with infinitely high walls, i.e., V = 0 for 0 < x < L, otherwise $V = \infty$. The normalized single particle energy eigenstates are

$$u_n(x) = \sqrt{\frac{2}{L}} \sin\left(n\pi x/L\right)$$

- (a) Find the wavefunctions and energies for the ground state and the first two excited states of the system.
- (b) Suppose that the two bosons interact with each other through the perturbing potential

$$H'(x_1, x_2) = -LV_0\delta(x_1 - x_2)$$

Compute the first-order correction to the ground state energy of the system.

12.9.2 Two Fermions in a Well

Two identical spin-1/2 bosons are placed in a 1-dimensional square potential well with infinitely high walls, i.e., V = 0 for 0 < x < L, otherwise $V = \infty$. The normalized single particle energy eigenstates are

$$u_n(x) = \sqrt{\frac{2}{L}} \sin\left(n\pi x/L\right)$$

- (a) What are the allowed values of the total spin angular momentum quantum number, J? How many possible values are there fore the z-component of the total angular momentum?
- (b) If single-particle spin eigenstates are denoted by $|\uparrow\rangle = u$ and $|\downarrow\rangle = d$, construct the two-particle spin states that are either symmetric or antisymmetric. How many states of each type are there?
- (c) Show that the j = 1, m = 1 state must be symmetric. What is the symmetry of the J = 0 state?
- (d) What is the ground-state energy of the two-particle system, and how does it depend on the overall spin state?

12.9.3 Two spin-1/2 particles

The Hamiltonian for two spin-1/2 particles, one with mass m_1 and the other with m_2 , is given by

$$\hat{H} = \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + V_a(r) + \left(\frac{1}{4} - \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2}\right) V_b(r)$$

where $|\vec{r}| = \vec{r}_1 - \vec{r}_2$, $|\vec{r}| = r$ and

$$V_a(r) = \begin{cases} 0 & \text{for } r < a \\ V_0 & \text{for } r > a \end{cases}, \quad V_b(r) = \begin{cases} 0 & \text{for } r < b \\ V_0 & \text{for } r > b \end{cases}$$

with b < a and V_0 very large (assume V_0 is infinite where appropriate) and positive.

- (a) Determine the normalized position-space energy eigenfunction for the ground state. What is the spin state of the ground state? What is the degeneracy?
- (b) What can you say about the energy and spin state of the first excited state? Does your result depend on how much larger a is than b? Explain.

12.9.4 Hydrogen Atom Calculations

We discuss here some useful tricks for evaluating the expectation values of certain operators in the eigenstates of the hydrogen atom.

(a) Suppose we want to determine $\langle 1/r \rangle_{n\ell m}$. We can interpret $\langle \lambda/r \rangle_{n\ell m}$ as the 1^{st} -order correction due to the perturbation λ/r (same dependence on r as the potential energy). Show that this problem can be solved exactly by just replacing e^2 by $e^2 - \lambda$ everywhere in the original solution. So, the exact energy is

$$E(\lambda) = -\frac{m\left(e^2 - \lambda\right)^2}{2n^2\hbar^2}$$

the 1^{st} -order correction is the term linear in λ , that is,

$$E^{(1)} = \frac{me^2\lambda}{n^2\hbar^2} = \langle \lambda/r \rangle_{n\ell m}$$

Therefore we get

$$\langle 1/r \rangle_{n\ell m} = \frac{me^2}{n^2\hbar^2} = \frac{1}{n^2a_0}$$

We note (for later use) that

$$E(\lambda) = E^{(0)} + E^{(1)} + \dots = E(\lambda = 0) + \lambda \left(\frac{dE}{d\lambda}\right)_{\lambda=0} + \dots$$

so that one way to extract $E^{(1)}$ from the exact answer is to calculate

$$\lambda \left(\frac{dE}{d\lambda}\right)_{\lambda=0}$$

(b) Evaluate, in a manner similar to part (a), $\left<\vec{p}^2/2\mu\right>_{n\ell m}$ by considering the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{Ze^2}{r} + \lambda \frac{\hat{p}^2}{2\mu}$$

(c) Consider now $\langle \lambda/r^2 \rangle_{n\ell m}$. In this case, an exact solution is possible since the perturbation just modifies the centrifugal term as follows:

$$\frac{\hbar^2 \ell(\ell+1)}{2mr^2} + \frac{\lambda}{r^2} = \frac{\hbar^2 \ell'(\ell'+1)}{2mr^2}$$

where ℓ' is a function of λ . Now go back to the original hydrogen atom solution and show that the dependence of E on $\ell'(\lambda)$ is

$$E(\ell') = -\frac{mZ^2 e^4}{2\hbar^2 (k+\ell'+1)^2} = E(\lambda) = E^{(0)} + E^{(1)} + \dots$$

Then show that

$$\left\langle \lambda/r^2 \right\rangle_{n\ell m} = E^{(1)} \lambda \left(\frac{dE}{d\lambda}\right)_{\lambda=0} = \lambda \left(\frac{dE}{d\ell'}\right)_{\ell'=\ell} \left(\frac{d\ell'}{d\lambda}\right)_{\ell'=\ell}$$
$$= \frac{\lambda}{n^3 a_0^2 (\ell+1/2)}$$

or

$$\langle 1/r^2 \rangle_{n\ell m} = \frac{1}{n^3 a_0^2 (\ell + 1/2)}$$

(d) Finally consider $\langle \lambda/r^3 \rangle_{n\ell m}$. Since there is no such term in the hydrogen Hamiltonian, we resort to different trick. Consider the radial momentum operator

$$p_r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

Show that in terms of this operator we may write the radial part of the Hamiltonian

$$-\frac{\hbar^2}{2m} \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right)$$
$$\frac{p_r^2}{2m}$$

Now show that

as

$$\langle [H, p_r] \rangle = 0$$

in the energy eigenstates. Using this fact, and by explicitly evaluating the commutator, show that

$$\left\langle 1/r^3\right\rangle_{n\ell m} = \frac{Z}{a_0\ell(\ell+1)} \left\langle 1/r^2\right\rangle_{n\ell m}$$

and hence

$$\left< 1/r^3 \right>_{n\ell m} = \frac{Z^3}{n^3 a_0^3 \ell(\ell+1)(\ell+1/2)}$$

12.9.5 Hund's rule

Explain on the basis of Hund's rules why the ground state of carbon is ${}^{3}P_{0}$ and that of oxygen is ${}^{3}P_{2}$.

12.9.6 Russell-Saunders Coupling in Multielectron Atoms

Consider a configuration of k equivalent p electrons outside a closed shell, which we denote simply by p^k , i.e., carbon= p^2 , nitrogen= p^3 and oxygen= p^4 .

- (a) Use the implied-terms method to determine all the terms that can arise from p^3 . Which of them will have the lowest energy?
- (b) Repeat this calculation for p^4 and show that we get the same result as for p^2

12.9.7 Magnetic moments of proton and neutron

The magnetic dipole moment of the proton is

$$\hat{\mu}_p = g_p \frac{e}{2m_p} \hat{S}_p$$

with a measured magnitude corresponding to a value for the gyromagnetic ratio of

$$g_p = 2 \times (2.792847337 \pm 0.00000029)$$

We have not studied the Dirac equation yet, but the prediction of the Dirac equation for a point spin-1/2 particle is $g_p = 2$. We can understand the fact that the proton gyromagnetic ratio is not two as being due its compositeness, i.e., in a simple quark model, the proton is made up of three quarks, two *ups* (u), and a *down* (d). The quarks are supposed to be point spin-1/2, hence, their gyromagnetic ratios should be $g_u = g_d = 2$ (up to higher order corrections, as in the case of the electron). Let us see if we can make sense out of the proton magnetic moment.

The proton magnetic moment should be the sum of the magnetic moments of its constituents, and any moments due to their orbital motion in the proton. The proton is the ground state baryon, so we assume that the three quarks are bound together (by the strong interaction) in a state with no orbital angular momentum. The Pauli principle says that the two identical up quarks must have an overall odd wave function under interchange of all quantum numbers. We must apply this rule with some care since we will be including *color* as one of these quantum numbers.

Let us look at some properties of *color*. It is the strong interaction analog of electric charge in the electromagnetic interaction. However, instead of one fundamental dimension in charge, there are three color directions, labeled as *red* (r), *blue* (b), and *green* (g). Unitary transformations in this color space(up to overall phases) are described by elements of the group SU(3), the group of unimodular 3×3 matrices (electromagnetic charge corresponds to the group U(1) whose elements are local phase changes). Just like combining spins, we can combine these three colors according to a Clebsch-Gordon series, with the result

$$3 \otimes 3 \otimes 3 = 10 \oplus 8 \oplus 8 \oplus 1$$

These are different rules than for the addition of spin case because that case uses the rotation group instead. We do not need to understand all aspects of the SU(3) group for this problem. The essential aspect here is that there is a singlet in the decomposition, i.e., it is possible to combine three colors in a way as to get a color singlet state or a state with no net color charge. These turn out to be the states of physical interest for the observed baryons according to a postulate of the quark model.

- (a) The singlet state in the decomposition above must be antisymmetric under the interchange of any two colors. Assuming this is the case, write down the color portion of the proton wave function.
- (b) Now that you know the color wave function of the quarks in the proton, write down the spin wave function. You must construct a total spin state |1/2, 1/2) total spin angular momentum state from three spin-1/2 states where the two up quarks must be in a symmetric state.
- (c) Since the proton is und and its partner the neutron (the are just two states of the same particle) is ddu and $m_p \simeq m_n$, we can make the simplifying assumption that $m_u \simeq m_d$. Given the measured value of g_p , what does you model give for m_u ? Remember that the up quark has electric charge 2/3 and the down quark has electric charge -1/3, in units of positron charge.
- (d) Finally, use your results to predict the gyromagnetic moment of the neutron(neutron results follows from proton results by interchanging u and d labels) and compare with observation.

12.9.8 Particles in a 3-D harmonic potential

A particle of mass m moves in a 3-dimensional harmonic oscillator well. The Hamiltonian is

$$\hat{H} = \frac{\vec{p}^2}{2m} + \frac{1}{2}kr^2$$

- (a) Find the energy and orbital angular momentum of the ground state and the first three excited states.
- (b) If eight identical non-interacting (spin 1/2) particles are placed in such a harmonic potential, find the ground state energy for the eight-particle system.
- (c) Assume that these particles have a magnetic moment of magnitude μ . If a magnetic field *B* is applied, what is the approximate ground state energy of the eight-particle system as a function of *B* (what is the effect of a closed shell?). Determine the magnetization $-\partial E/\partial B$ for the ground state as a function of *B*. What is the susceptibility? Don't do any integrals.

12.9.9 2 interacting particles

Consider two particles of masses $m_1 \neq m_2$ interacting via the Hamiltonian

$$\hat{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m_1\omega^2 x_1^2 + \frac{1}{2}m_2\omega^2 x_2^2 + \frac{1}{2}K(x_1 - x_2)^2$$

- (a) Find the exact solutions.
- (b) Sketch the spectrum in weak coupling limit $K<<\mu\omega^2$ where μ = reduced mass.

12.9.10 LS versus JJ coupling

Consider a multielectron atom whose electron configuration is

$$1s^22s^22p^63s^23p^63d^{10}4s^24p4d$$

- (a) To what element does this configuration belong? Is it the ground state or an excited state? Explain.
- (b) Suppose that we apply the Russell-Saunders coupling scheme to this atom. Draw and energy level diagram roughly to scale for the atom, beginning with the single unperturbed configuration energy and taking into account the various interactions one at a time in the correct order. Be sure to label each level at each stage of your diagram with the appropriate term designation, quantum numbers and so on.
- (c) Suppose instead we apply pure jj-coupling to the atom. Starting again from the unperturbed n = 4 level, draw a second energy level diagram. [HINT: Assume that for a given level (j_1, j_2) , the state with the lowest Jlies lowest in energy]

12.9.11 In a harmonic potential

Two identical, noninteracting spin= 1/2 particles of mass m are in a one dimensional harmonic oscillator potential for which the Hamiltonian is

$$H = \frac{p_{1x}^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{p_{2x}^2}{2m} + \frac{1}{2}m\omega^2 x_2^2$$

- (a) Determine the ground-state and first-excited state kets and the corresponding energies when the two particles are in a total spin= 0 state. What are the lowest energy states and the corresponding kets for the particles if they are in a total spin= 1 state?
- (b) Suppose that the two particles interact with a potential energy of interaction

$$V(|x_1 - x_2|) = \begin{cases} -V_0 & |x_1 - x_2| < a \\ 0 & \text{elsewhere} \end{cases}$$

Argue what the effect will be on the energies that you determined in (a), that is, whether the energy of each state moves up, moves down, or remains unchanged.

12.9.12 2 particles interacting via delta function

Two particles of mass m are placed in a rectangular box of sides a > b > c in the lowest energy state of the system compatible with the conditions below. The particles interact with each other according to the potential $V = A\delta(\vec{r}_1 - \vec{r}_2)$. Using first order perturbation theory calculate the energy of the system under the following conditions:

- (a) particles are not identical
- (b) identical particles of spin= 0
- (c) identical particles of spin= 1/2 with spins parallel

12.9.13 2 particles in a square well

Two identical nonrelativistic fermions of mass m, spin= 1/2 are in a 1-dimensional square well of length L with V infinitely large outside the well. The fermions are subject to a repulsive potential $V(x_1 - x_2)$, which may be treated as a perturbation.

- (a) Classify the three lowest-energy states in terms of the states of the individual particles and state the spin of each.
- (b) Calculate to first-order the energies of the second- and third- lowest states; leave your result in the form of an integral. Neglect spin-dependent forces throughout.

12.9.14 2 particles interacting via a harmonic potential

Two particles, each of mass ${\cal M}$ are bound in a 1–dimensional harmonic oscillator potential

$$V = \frac{1}{2}kx^2$$

and interact with each other through an attractive harmonic force $F_{12} = -K(x_1 - x_2)$. Assume that K is very small.

- (a) What are the energies of the three lowest states of this system?
- (b) If the particles are identical and spinless, which of the states of (a) are allowed?
- (c) If the particles are identical and have spin= 1/2, which of the states of (a) are allowed?

12.9.15 The Structure of helium

Consider a Helium atom in the 1s2p configuration. The total angular momentum is L = 1 (a *P*-state). Due to the Fermi-Pauli symmetry this state splits into singlet and triplet multiplets as shown below.

where the superscripts 1 and 3 represent the spin degeneracy for the singlet/triplet respectively.

(a) Explain qualitatively why the triplet state has lower energy.

Now include spin-orbit coupling described by the Hamiltonian $\hat{H}_{SO} = f(r)\hat{L}\cdot\hat{S}$, where \hat{L} and \hat{S} are the total orbital and spin angular momentum respectively.



Figure 12.12: Fermi-Pauli Splittings

- (b) Without the spin-orbit interaction, good quantum numbers for the angular momentum degrees of freedom are $|LM_LSM_S\rangle$. What are the good quantum numbers with spin-orbit present?
- (c) The energy level diagram including spin-orbit corrections is sketched below.



Figure 12.13: Including Spin-Orbit

Label the states with appropriate quantum numbers. NOTE: Some of the levels are degenerate; the sublevels are not shown.

Chapter 13

Scattering Theory and Molecular Physics

13.1 Scattering Theory

One of the main techniques used by physicists to obtain information about the structure of all forms of matter from elementary particles to solids is the scattering of particles.

A *particle* is a localized region in space and time that contains energy and momentum. In quantum mechanics a good representation of a particle is a *wave packet* as we saw earlier. We will assume that the potential that is responsible for the scattering effects is of *short range* in space.

We also assume that the spatial extent of the wave packet is small compared to the spatial dimensions of the laboratory, i.e., the detectors , etc, but that it is large compared to the size of the scattering region.

We imagine an experimental setup as shown below in Figure 13.1:



Figure 13.1: Scattering Experimental setup

The incident wavepacket is emitted by a source at time t_0 in a region where the potential is zero (or negligible) and we detect the scattered wave packet (at the detector) in another region where the potential is zero (or negligible).

The wave packet representing the incident particle is given by the expression

$$\psi(\vec{r}, t_0) = \int \frac{d^3 \vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} a_{\vec{k}}$$
(13.1)

where $a_{\vec{k}}$ has a maximum near \vec{k}_0 . Our earlier stationary phase arguments then say that this wave packet (region in space and time where $|\psi|^2$ is nonzero) travels with a velocity(group) $\hbar \vec{k}_0/m$ towards the target.

The scattering problem is to determine

$$\psi(\vec{r}, t)$$
 = wave function at the time t
after the particle has interacted
with the target (and we are far
from the target once again)

The solution method is as follows:

1. We solve for the exact eigenstates $\psi_{\vec{k}}(\vec{r})$ of the potential $V(\vec{r})$ using the Schrodinger equation

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_{\vec{k}}\right)\psi_{\vec{k}}(\vec{r}) = V(\vec{r})\psi_{\vec{k}}(\vec{r})$$
(13.2)

where

$$E_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$$
(13.3)

and all values of $E_{\vec{k}} \ge 0$ are allowed eigenvalues.

2. These eigenstates are a complete set so we can always write

$$\psi(\vec{r}, t_0) = \int \frac{d^3 \vec{k}}{(2\pi)^3} \psi_{\vec{k}}(\vec{r}) b_{\vec{k}}$$
(13.4)

where

$$\frac{\hbar^2 k^2}{2m} \ge 0 \tag{13.5}$$

for all the $\psi_{\vec{k}}(\vec{r})$ in the expansion.

These assumptions imply that only the incident (incoming) and scattered(outgoing) waves appear and that no bound state contribute since they would have E < 0 and thus fall off exponentially. 3. Since we now have an expansion in energy eigenstates it is trivial to incorporate the time evolution of $\psi(\vec{r}, t)$. We get

$$\psi(\vec{r},t) = \int \frac{d^3\vec{k}}{(2\pi)^3} \psi_{\vec{k}}(\vec{r}) b_{\vec{k}} e^{-i\frac{E_{\vec{k}}}{\hbar}(t-t_0)}$$
(13.6)

This is the formal solution to the scattering problem.

13.1.1 Green's Functions

We now need to determine the exact eigenstates $\psi_{\vec{k}}(\vec{r})$. We will use a Green's function approach similar to the one we introduced earlier for 1-dimensional transmission/reflection problems.

The Green's function for the free particle Schrodinger equation is given by the differential equation

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_{\vec{k}}\right)G(\vec{r},k) = \delta(\vec{r})$$
(13.7)

In terms of this function, the solution to the full Schrodinger equation is

$$\psi_{\vec{k}}(\vec{r}) = \phi_0(\vec{r}) + \int d^3 \vec{r}' G(\vec{r} - \vec{r}', k) V(\vec{r}') \psi_{\vec{k}}(\vec{r}')$$
(13.8)

where

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_{\vec{k}}\right)\phi_0(\vec{r}) = 0 \tag{13.9}$$

and $\phi_0(\vec{r})$ is the free-particle wave function (solution of the homogenous equation that results when V = 0). We then have

$$\phi_0(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \tag{13.10}$$

Direct substitution shows that we have a general solution to the Schrödinger equation.

$$\begin{pmatrix} \frac{\hbar^2}{2m} \nabla^2 + E_{\vec{k}} \end{pmatrix} \psi_{\vec{k}}(\vec{r}) = \left(\frac{\hbar^2}{2m} \nabla^2 + E_{\vec{k}} \right) \phi_0(\vec{r})$$

+ $\int d^3 \vec{r}' \left(\frac{\hbar^2}{2m} \nabla^2 + E_{\vec{k}} \right) G(\vec{r} - \vec{r}', k) V(\vec{r}') \psi_{\vec{k}}(\vec{r}')$
= $\int d^3 \vec{r}' \delta(\vec{r} - \vec{r}') V(\vec{r}') \psi_{\vec{k}}(\vec{r}') = V(\vec{r}) \psi_{\vec{k}}(\vec{r})$

How do we interpret this solution in the context of the scattering problem?

We identify the following terms

$$\phi_0(\vec{r}) = \text{ incident wave}$$
$$\int d^3\vec{r}' G(\vec{r} - \vec{r}', k) V(\vec{r}') \psi_{\vec{k}}(\vec{r}') = \text{ scattered wave}$$

In addition, we then say

$$V(\vec{r}')\psi_{\vec{k}}(\vec{r}') = \text{potential} \times \text{amplitude evaluated at } \vec{r}'$$

= source of the scattered wave
$$G(\vec{r} - \vec{r}', k) = \text{amplitude of the scattered wave at } \vec{r} \text{ due}$$

to a unit source $(\delta(\vec{r}'))$ at \vec{r}'

The integral is then the total scattered wave (adds up all waves coming from all parts of the target region) and is equal to the sum over all source points \vec{r}' .

For this interpretation to make physical sense $G(\vec{r} - \vec{r}', k)$ must generate *outgo-ing waves only*!

We can determine the Green's function, as we did earlier, using Fourier transforms and complex contour integration. As before, the choice of the contour will be equivalent to choosing boundary conditions for the differential equation and thus completing the solution of the problem.

In this case we must choose a boundary condition (contour of integration) that generates outgoing waves *only*.

Let us now determine the Green's function and do the integrals.

We write (using Fourier transforms)

$$G(\vec{r},k) = \int \frac{d^3 \vec{p}}{(2\pi)^3} e^{i\vec{p}\cdot\vec{r}} \tilde{G}(\vec{p})$$
(13.11)

$$\delta(\vec{r}) = \int \frac{d^3 \vec{p}}{(2\pi)^3} e^{i \vec{p} \cdot \vec{r}}$$
(13.12)

Substitution then gives

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_{\vec{k}}\right) G(\vec{r},k) = \int \frac{d^3\vec{p}}{(2\pi)^3} \left(\frac{\hbar^2}{2m}\nabla^2 + E_{\vec{k}}\right) e^{i\vec{p}\cdot\vec{r}} \tilde{G}(\vec{p})$$

$$= \int \frac{d^3\vec{p}}{(2\pi)^3} \left(-\frac{\hbar^2 p^2}{2m} + \frac{\hbar^2 k^2}{2m}\right) e^{i\vec{p}\cdot\vec{r}} \tilde{G}(\vec{p})$$

$$= \int \frac{d^3\vec{p}}{(2\pi)^3} e^{i\vec{p}\cdot\vec{r}}$$
(13.13)

This implies that

$$\tilde{G}(\vec{p}) = \frac{1}{\frac{\hbar^2}{2m} \left(k^2 - p^2\right)}$$
(13.14)

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Therefore, we obtain

$$G(\vec{r},k) = \int \frac{d^{3}\vec{p}}{(2\pi)^{3}} e^{i\vec{p}\cdot\vec{r}} \frac{1}{\frac{\hbar^{2}}{2m} (k^{2} - p^{2})}$$

$$= -\frac{2m}{8\pi^{3}\hbar^{2}} \int_{0}^{2\pi} d\varphi \int_{-1}^{1} d\cos\theta \int_{0}^{\infty} \frac{e^{ipr\cos\theta}}{p^{2} - k^{2}} p^{2} dp$$

$$= -\frac{m}{2\pi^{2}\hbar^{2}} \frac{1}{ir} \int_{0}^{\infty} \frac{p}{p^{2} - k^{2}} dp \int_{-ipr}^{ipr} dx e^{x}$$

$$= -\frac{m}{2\pi^{2}\hbar^{2}} \frac{1}{ir} \int_{0}^{\infty} \frac{p}{p^{2} - k^{2}} \left(e^{ipr} - e^{-ipr}\right) dp$$

$$= -\frac{m}{2\pi^{2}\hbar^{2}} \frac{1}{ir} \int_{-\infty}^{\infty} \frac{pe^{ipr}}{p^{2} - k^{2}} dp \qquad (13.15)$$

The integrand has poles at $p=\pm k.$ If we choose a contour as shown in Figure 13.2 below



Figure 13.2: Integration Contour

then we have

$$-\frac{m}{2\pi^2\hbar^2} \frac{1}{ir} \left[\int_{-\infty}^{\infty} \frac{pe^{ipr}}{p^2 - k^2} dp + \int_{semicircle} \frac{ze^{izr}}{z^2 - k^2} dz \right] = 2\pi i \text{Residue}(+k)$$

Now

$$\int_{semicircle} \frac{ze^{izr}}{z^2 - k^2} dz \to 0 \text{ as the radius of the semicircle } \to \infty$$
(13.16)

due to the e^{ipr} term which behaves like $e^{-Imag(p)r} \to 0$ if Imag(p) > 0 as it does on contour C.

The residue at +k is

$$\frac{ke^{ikr}}{2k} = \frac{e^{ikr}}{2} \tag{13.17}$$

Therefore,

$$G(\vec{r},k) = -\frac{m}{2\pi^2\hbar^2} \frac{1}{ir} 2\pi i \frac{e^{ikr}}{2} = -\frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r}$$
(13.18)

This physically represents an outgoing spherical wave as is required by the boundary conditions of the scattering problem.

Putting everything together we have

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{m}{2\pi\hbar^2} \int d^3\vec{r}' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}')\psi_{\vec{k}}(\vec{r}')$$
(13.19)

Note that since the time dependence of $\psi_{\vec{k}}(\vec{r}')$ is $e^{-iE_{\vec{k}}t/\hbar}$, we are adding up terms of the form

$$\frac{e^{i(k|\vec{r}-\vec{r}\,'|-\frac{E_{\vec{k}}}{\hbar}\,t)}}{|\vec{r}-\vec{r}\,'|} \tag{13.20}$$

which are outgoing waves with the appropriate inverse square relationship built in!

The magnitude of the outgoing momentum is

 $\hbar k$ = same as the incoming momentum

(only the direction has changed)

Therefore, potential scattering of this type is elastic scattering.

Since we are assuming that the detectors are far away from the target, we can look at solutions where $|\vec{r}| \gg |\vec{r}'|$. In this case, we have

$$k |\vec{r} - \vec{r}'| = k \sqrt{(\vec{r} - \vec{r}') \cdot (\vec{r} - \vec{r}')} = k \left(r^2 + r'^2 - 2\vec{r} \cdot \vec{r}'\right)^{1/2}$$

$$\approx k \left(r^2 - 2\vec{r} \cdot \vec{r}'\right)^{1/2} = kr \left(1 - 2\frac{\vec{r}}{r} \cdot \vec{r}'\right)^{1/2}$$

$$\approx kr \left(1 - \frac{\vec{r}}{r} \cdot \vec{r}'\right) = kr - \vec{k}' \cdot \vec{r}'$$
(13.21)

where

$$\vec{k}' = k\hat{r} = k\frac{\dot{r}}{r} =$$
 wave vector seen at the detector (13.22)

Therefore, at the detector we have

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r} f_{\vec{k}}(\theta,\varphi)$$
(13.23)

where
$$(\theta, \varphi)$$
 = direction of *vecr* and

$$f_{\vec{k}}(\theta,\varphi) = -\frac{m}{2\pi\hbar^2} \int d^3\vec{r}' e^{-i\vec{k}\cdot\vec{r}'} V(\vec{r}')\psi_{\vec{k}}(\vec{r}')$$
(13.24)

= the scattering amplitude

The term

$$\frac{e^{ikr}}{r}f_{\vec{k}}(\theta,\varphi) \tag{13.25}$$

implies

$$\begin{array}{l} \text{amplitude that particle}\\ \text{will reach } r \text{ after being}\\ \text{scattered at the target-}\\ \text{outgoing wave + inverse}\\ r-\text{squared effect} \end{array} \right) \times \left(\begin{array}{c} \text{amplitude that incident}\\ \text{particle will be scattered}\\ \text{with } k \text{ in the direction}\\ (\theta, \varphi) \end{array}\right)$$
(13.26)

Using the exact solution for $\psi_{\vec{k}}(\vec{r})$

$$\psi_{\vec{k}}(\vec{r}) + \frac{m}{2\pi\hbar^2} \int d^3\vec{r}' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi_{\vec{k}}(\vec{r}') = e^{i\vec{k}\cdot\vec{r}}$$
(13.27)

we can substitute for $e^{i\vec{k}\cdot\vec{r}}$ to get

$$\psi(\vec{r},t_0) = \int \frac{d^3\vec{k}}{(2\pi)^3} \left[\psi_{\vec{k}}(\vec{r}) + \frac{m}{2\pi\hbar^2} \int d^3\vec{r}' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}')\psi_{\vec{k}}(\vec{r}') \right] a_{\vec{k}} \quad (13.28)$$

Now we assumed that $a_{\vec{k}}$ has a maximum near \vec{k}_0 which implies that inside the brackets [....] we can write $\psi_{\vec{k}}(\vec{r}\,') \approx \psi_{\vec{k}_0}(\vec{r}\,')$ and since $k_0 \gg |\vec{k} - \vec{k}_0|$ we get

$$k = \frac{\vec{k} \cdot \vec{k}}{k} \approx \frac{\vec{k}_0 \cdot \vec{k}}{k_0} = \hat{k}_0 \cdot \vec{k}$$
(13.29)

Therefore, the last term becomes

$$\int \frac{d^3\vec{k}}{(2\pi)^3} a_{\vec{k}} e^{i\vec{k}\cdot\hat{k}_0|\vec{r}-\vec{r}\,'|} \psi_{\vec{k}_0}(\vec{r}\,') = \psi(\hat{k}_0\,|\vec{r}-\vec{r}\,'|\,,t_0) \psi_{\vec{k}_0}(\vec{r}\,') = 0 \tag{13.30}$$

This is zero because at $t = t_0$, $\psi(\hat{k}_0 | \vec{r} - \vec{r'} |, t_0) = 0$ since $\hat{k}_0 | \vec{r} - \vec{r'} |$ is to the right of the potential.

Therefore,

$$\psi(\vec{r}, t_0) = \int \frac{d^3\vec{k}}{(2\pi)^3} \psi_{\vec{k}}(\vec{r}) a_{\vec{k}}$$
(13.31)

which implies $a_{\vec{k}} = b_{\vec{k}}$, i.e., the expansion coefficients are the same whether we expand in plane waves or the exact energy eigenstates.

Thus, we can write

$$\psi(\vec{r},t) = \int \frac{d^3\vec{k}}{(2\pi)^3} \psi_{\vec{k}}(\vec{r}) a_{\vec{k}} e^{-i\frac{E_{\vec{k}}}{\hbar}(t-t_0)}$$
(13.32)

For \vec{r} far from the target, we can use the asymptotic form for $\psi_{\vec{k}}(\vec{r})$ to get

$$\psi(\vec{r},t) = \psi_0(\vec{r},t) + \int \frac{d^3\vec{k}}{(2\pi)^3} a_{\vec{k}} \frac{e^{i\left(\vec{k}\cdot\vec{r} - \frac{E_{\vec{k}}}{\hbar}(t-t_0)\right)}}{r} f_{\vec{k}}(\theta,\varphi)$$
(13.33)

where

$$\psi_0(\vec{r},t) = \int \frac{d^3\vec{k}}{(2\pi)^3} a_{\vec{k}} \frac{e^{i\left(\vec{k}\cdot\vec{r}-\frac{E_{\vec{k}}}{\hbar}(t-t_0)\right)}}{r}$$

$$= \text{ wave packet at time } t \text{ if } V = 0$$
(13.34)

Finally, putting in the approximations

$$f_{\vec{k}} \approx f_{\vec{k}_0} \text{ and } k \approx \vec{k} \cdot \hat{k}_0$$
 (13.35)

we get

$$\psi(\vec{r},t) = \psi_0(\vec{r},t) + \frac{f_{\vec{k}_0}(\theta,\varphi)}{r} \psi_0(\hat{k}_0 r,t)$$
(13.36)

The meaning of these terms is as follows:

- 1. $\psi(\vec{r}, t) =$ (no scattering term) + (scattered wave)
- 2. the scattered term includes

$$\begin{split} \psi_0(\hat{k}_0r,t) &= \text{ amplitude to be at } \hat{k}_0r \text{ at time } t \\ &= \text{value of wave function at this point;} \\ & \text{ all the potential did was to bend the } \\ & \text{ particle path towards } \vec{r} \\ \hline \frac{f_{\vec{k}_0}(\theta,\varphi)}{r} &\to \text{ probability amplitude that the } \end{split}$$

This result fails

- 1. if a scattering resonance is present since this implies that the wave packet experiences strong deformations
- 2. if the potential has a long range effect

13.1.2 Cross Sections

The quantity used to connect theory to experiment in scattering experiments is the differential scattering cross section.

It is defined as follows: if

- 1. N_{in} = number of incident particles per cm^2
- 2. $dN(\theta, \varphi)$ = number of particles scattered in ot a solid angle $d\Omega$ centered at (θ, φ)

then

$$\frac{d\sigma}{d\Omega} = \frac{dN(\theta,\varphi)}{N_{in}d\Omega}$$
(13.37)

In terms of a single particle, $d\sigma/d\Omega$ is the total probability that the particle is scattered into a unit solid angle divided by the total probability that the particle crosses a unit area in front of the target.

The same assumptions are made as earlier, i.e., the incident packet size \gg size of the target and the detector is far from the incident bean and the target.

Now the total probability of being scattered into an infinitesimal solid angle $d\Omega$ at \vec{r} is the rate that probability strikes an area $r^2 d\Omega$ in the detector plane integrated over time.

This is given by

$$\int_{-\infty}^{\infty} dt \times (\text{velocity}) \times (\text{area at detector}) \times (\text{probability of scattering})$$
$$= \int_{-\infty}^{\infty} dt \times \left(\frac{\hbar k_0}{m}\right) \times \left(r^2 d\Omega\right) \times \frac{\left|f_{\vec{k}_0}(\theta,\varphi)\right|^2}{r^2} \left|\psi_0(\hat{k}_0 r, t)\right|^2 \tag{13.38}$$

or the total probability of being scattered into $d\Omega$ is

$$\left|f_{\vec{k}_{0}}(\theta,\varphi)\right|^{2}d\Omega\left[\frac{\hbar k_{0}}{m}\int_{-\infty}^{\infty}dt\left|\psi_{0}(\hat{k}_{0}r,t)\right|^{2}\right]$$
(13.39)

The total probability that crosses a unit area at \vec{r}_0 in front of the target in the incident beam is

$$\int_{-\infty}^{\infty} dt (\text{probability flux}) = \frac{\hbar k_0}{m} \int_{-\infty}^{\infty} dt \left| \psi_0(\hat{k}_0 r, t) \right|^2$$
(13.40)

If we assume that the wave packet does not spread between \vec{r}_0 and $\vec{k}_0 r$ (this just says a particle remains a particle during the duration of the experiment), then we have

$$\frac{d\sigma}{d\Omega} = \text{ ratio of these last two terms } = \left| f_{\vec{k}_0}(\theta, \varphi) \right|^2$$
(13.41)

This result does not depend on the details of the incident wave packet.

Finally, the total cross section σ , where

$$\sigma = \int_{\substack{\text{all}\\\text{solid}\\\text{angles}}} \frac{d\sigma}{d\Omega} d\Omega$$
(13.42)

= total probability of being scattered divided by the

total probability that the particle crossed a unit area

in front of the target

$$= \int d\Omega \left| f_{\vec{k}_0}(\theta, \varphi) \right|^2 \tag{13.43}$$

Since experimentalists can measure σ and $d\sigma/d\Omega$, the theorist needs to be able to calculate them given the potential function.

13.1.3 Partial Waves

We now look at the special case where $V(\vec{r}) = V(r)$ is spherically symmetric. In this case, the angular momentum of the incident particle is conserved, i.e.,

$$\left[\hat{H}, \vec{L}_{op}^{2}\right] = 0 = \left[\hat{H}, \hat{L}_{z}\right]$$
 (13.44)

This means we should only consider stationary state solutions that are also eigenstates of the angular momentum.

We start off with an identity (see Addition Theorem discussion in Chapter 12). If we choose $\vec{k}=k\hat{z},$ then we can write

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\theta} = e^{ikz} = \sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1)P_{\ell}(\cos\theta)j_{\ell}(kr)$$
(13.45)

This is an expansion of a plane wave in spherical harmonics (or angular momentum eigenfunctions). The expansion coefficients are spherical Bessel functions. Physically, the expansion implies that an plane wave of infinite spatial extent contains all possible orbital angular momentum values.

In this expansion

$$P_{\ell}(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell 0}(\theta,\varphi)$$
(13.46)

= Legendre polynomial of order ℓ

and

$$j_{\ell}(kr) = \frac{1}{2} \left(h_{\ell}(kr) + h_{\ell} * (kr) \right)$$
(13.47)

where the $h_{\ell}(kr)$ are Hankel functions.

Since the incident plane wave is independent of φ (rotation about the direction

of \vec{k}), the scattered wave must be invariant under rotations about the direction of \vec{k}' , which implies that

$$f_{\vec{k}}(\theta,\varphi) \to f_{\vec{k}}(\theta)$$
 (13.48)

For functions of θ , the Legendre polynomials are a complete set so we can expand $f_{\vec{k}}(\theta)$ as

$$f_{\vec{k}}(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell} P_{\ell}(\cos\theta)$$
(13.49)

Each ℓ term is called a partial wave and f_ℓ is the partial wave scattering amplitude.

For similar reasons, the stationary state wave functions can be written as

$$\psi_{\vec{k}}(\vec{r}) = \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) P_{\ell}(\cos\theta) R_{\ell}(r)$$
(13.50)

where

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right) r R_\ell(r) = \frac{2m}{\hbar^2} V(r) r R_\ell(r)$$
(13.51)

In the limit of large r (where the detector is located), assuming that $r^2 V(r) \rightarrow 0$, we get

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right) r R_\ell(r) = 0$$
(13.52)

which is Bessel's equation.

Therefore, near the detector $(r \to \infty)$ we can write $R_{\ell}(r)$ as a linear combination of the $h_{\ell}(kr)$ and $h_{\ell}^*(kr)$. In particular, we assume the form

$$R_{\ell}(r) = B_{\ell} \left[h_{\ell} * (kr) + S_{\ell}(E) h_{\ell}(kr) \right]$$
(13.53)

The $h_{\ell}^*(kr)$ term represents an incoming spherical wave and the $h_{\ell}(kr)$ term represents an outgoing spherical wave. We have therefore assumed that the effect of the potential will be to modify only the outgoing wave.

In the absence of scattering, i.e., V = 0, we have

$$R_{\ell}(r) = j_{\ell}(kr) = \frac{1}{2} \left[h_{\ell} * (kr) + h_{\ell}(kr) \right]$$
(13.54)

which implies that

$$B_{\ell} = \frac{1}{2} \text{ and } S_{\ell} = 1$$
 (13.55)

When $V(r) \neq 0$ only S_{ℓ} changes.

We will be considering only elastic scattering in this discussion.

In the Schrodinger picture, we can talk about probability densities and probability flows or currents. In non-relativistic quantum mechanics we have a probability interpretation for the wave function which implies that

probability density =
$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2$$
 (13.56)

and

.

$$\int |\psi(\vec{r},t)|^2 d^3 \vec{r} = 1$$
(13.57)

Since there are no sources or sinks of probability in non-relativistic quantum mechanics (no particle creation or annihilation processes) we must have a continuity equation of the form

$$\frac{\partial P}{\partial t} + \nabla \cdot \vec{J} = 0 \tag{13.58}$$

where

$$\vec{J}$$
 = probability current (13.59)

Using (13.56) and the time-dependent Schrödinger equation we get

$$\vec{J} = \frac{\hbar}{2im} \left[\psi * \nabla \psi - \psi \nabla \psi * \right]$$
(13.60)

Proof:

$$\begin{split} i\hbar\frac{\partial P}{\partial t} &= i\hbar\frac{\partial}{\partial t}\left|\psi(\vec{r},t)\right|^2 = i\hbar\frac{\partial\psi^*}{\partial t}\psi + i\hbar\psi*\frac{\partial\psi}{\partial t} \\ &= \left(-\frac{\hbar^2}{2m}\nabla^2\psi*+V\psi*\right)\psi+\psi*\left(\frac{\hbar^2}{2m}\nabla^2\psi-V\psi\right) \\ &= \frac{\hbar}{2im}\left[\psi*\nabla^2\psi-\psi\nabla^2\psi*\right] = -\frac{\hbar}{2im}\nabla\cdot\left[\psi*\nabla\psi-\psi\nabla\psi*\right] \\ &= -\nabla\cdot\vec{J} \end{split}$$

Since as many particles enter a sphere of radius r surrounding the target as leave the sphere (this is the meaning of elastic scattering), the radial component of the current must be zero or

$$J_r(r) = \frac{\hbar}{2im} \left[R_\ell * (r) \frac{\partial R_\ell(r)}{\partial r} - R_\ell(r) \frac{\partial R_\ell * (r)}{\partial r} \right] = 0$$
(13.61)

Substitution of (13.53) implies that we must have

$$|S_{\ell}(E)| = 1 \tag{13.62}$$

which says that we can always write

$$S_{\ell}(E) = e^{2i\delta_{\ell}(E)}$$
 where δ_{ℓ} is real (13.63)

 δ_{ℓ} is called the phase shift and $2\delta_{\ell}$ equals the difference in phase between the outgoing parts of the wave function $\psi_{\vec{K}}(\vec{r})$ and the incident plane wave $e^{i\vec{k}\cdot\vec{r}}$.

The phase shift contains the all of the effects of the potential on the wave function.

Since the $\delta_{\ell}(E)$ are constants for a given scattering process (since E = constant), we can determine their values at any point in the scattering process.

Let us look at r very large where V(r) = 0. We can then write

$$\begin{split} \psi_{\vec{k}}(\vec{r}) &= \frac{1}{2} \sum_{\ell} i^{\ell} (2\ell+1) P_{\ell}(\cos \theta) \left[h_{\ell} * (kr) + e^{2i\delta_{\ell}} h_{\ell}(kr) \right] \\ &= \frac{1}{2} \sum_{\ell} i^{\ell} (2\ell+1) P_{\ell}(\cos \theta) \left[h_{\ell} * (kr) + h_{\ell}(kr) + (e^{2i\delta_{\ell}} - 1) h_{\ell}(kr) \right] \\ &= \frac{1}{2} \sum_{\ell} i^{\ell} (2\ell+1) P_{\ell}(\cos \theta) \left[h_{\ell} * (kr) + h_{\ell}(kr) \right] \\ &\quad + \frac{1}{2} \sum_{\ell} i^{\ell} (2\ell+1) P_{\ell}(\cos \theta) \left[(e^{2i\delta_{\ell}} - 1) h_{\ell}(kr) \right] \\ &= \sum_{\ell} i^{\ell} (2\ell+1) P_{\ell}(\cos \theta) j_{\ell}(kr) \\ &\quad + \frac{1}{2} \sum_{\ell} i^{\ell} (2\ell+1) P_{\ell}(\cos \theta) \left[(e^{2i\delta_{\ell}} - 1) h_{\ell}(kr) \right] \\ &= e^{i\vec{k}\cdot\vec{r}} + \frac{1}{2} \sum_{\ell} i^{\ell} (2\ell+1) P_{\ell}(\cos \theta) \left[(e^{2i\delta_{\ell}} - 1) h_{\ell}(kr) \right] \end{split}$$
(13.64)

But we know that

$$h_{\ell}(kr) \to \frac{e^{i(kr - \frac{\ell\pi}{2})}}{ikr} \text{ as } r \to \infty$$
 (13.65)

Substituting this result and using

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \frac{f(\theta)}{r}e^{ikr}$$

we get

$$f(\theta) = \frac{1}{2ik} \sum_{\ell} (2\ell+1) P_{\ell}(\cos\theta) \left(e^{2i\delta_{\ell}} - 1\right)$$
(13.66)

$$= \frac{1}{k} \sum_{\ell} (2\ell + 1) P_{\ell}(\cos \theta) e^{i\delta_{\ell}} \sin \delta_{\ell}$$
(13.67)

where

$$f_{\ell} = e^{2i\delta_{\ell}} - 1 = e^{i\delta_{\ell}} \sin \delta_{\ell} \tag{13.68}$$

= the partial wave scattering amplitude

We obtain the total cross section using

$$\sigma = \int |f(\theta)|^2 d\Omega \tag{13.69}$$
$$= \sum_{\ell} \sum_{\ell'} \frac{(2\ell+1)}{k} \frac{(2\ell'+1)}{k} e^{-i\delta_{\ell}} e^{i\delta_{\ell'}} \sin \delta_{\ell} \sin \delta_{\ell'} \int_{0}^{2\pi} d\varphi \int_{-1}^{1} dx P_{\ell}(x) P_{\ell'}(x)$$

Now

$$\int_{-1}^{1} dx P_{\ell}(x) P_{\ell'}(x) = \frac{\delta_{\ell\ell'}}{2\ell + 1}$$
(13.70)

which implies that

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell} \left(2\ell + 1\right) \sin^2 \delta_{\ell} = \sum_{\ell} \sigma_{\ell} \tag{13.71}$$

where

$$\sigma_{\ell} = \frac{4\pi}{k^2} (2\ell + 1) \sin^2 \delta_{\ell} \tag{13.72}$$

is the partial wave cross section for scattering particles in angular momentum $\ell\text{-states.}$

Since $\sin^2 \delta_{\ell} \leq 1$, we have the limit

$$\sigma_{\ell} \le \frac{4\pi}{k^2} (2\ell + 1) \tag{13.73}$$

Classically, the maximum ℓ value that contributes to the sum is given by

$$\ell_{\max} = ka \tag{13.74}$$

where a is the range of the potential (i.e., for, V(r) = 0 we have no scattering).

Quantum mechanically, for r > a, only the term

$$\frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$
(13.75)

acts. For energy

$$E = \frac{\hbar^2 k^2}{2m} \tag{13.76}$$

the classical turning radius is

$$r_{cl} = \frac{\sqrt{\ell(\ell+1)}}{k} \tag{13.77}$$

For $r < r_{cl}$, the wave function falls off exponentially. If $r_{cl} > a$, then the particle *feels* nothing from the potential, which says that the particle is scattered only if

$$r_{cl} \le a \text{ or } \sqrt{\ell(\ell+1)} \approx \ell \le ka$$
 (13.78)

Note that there are interference effects between different partial waves $d\sigma/d\Omega$ but not in σ .

13.1.4 The Optical Theorem

We earlier derived the relations

$$f(\theta) = \frac{1}{k} \sum_{\ell} (2\ell + 1) P_{\ell}(\cos \theta) e^{i\delta_{\ell}} \sin \delta_{\ell}$$
(13.79)

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell} \left(2\ell + 1\right) \sin^2 \delta_{\ell} \tag{13.80}$$

These lead to another important result.

$$Imag(f(\theta)) = \frac{1}{k} \sum_{\ell} (2\ell + 1) P_{\ell}(\cos\theta) \sin^2 \delta_{\ell}$$
(13.81)

$$Imag(f(0)) = \frac{1}{k} \sum_{\ell} (2\ell + 1) P_{\ell}(1) \sin^2 \delta_{\ell} = \frac{1}{k} \sum_{\ell} (2\ell + 1) \sin^2 \delta_{\ell}$$
(13.82)

or

$$\sigma = \frac{4\pi}{k} Imag(f(0)) \tag{13.83}$$

which is the *optical theorem*.

13.1.5 Born Approximation

In some special cases, i.e., special potential functions, large ℓ or sma;; k for $\ell \ge 1$, we can find an approximate analytic expression for δ_{ell} . In general, however, we must solve the problem numerically.

One such analytical method goes as follows.

We have the general relations

$$f_{\vec{k}}(\theta,\varphi) = -\frac{m}{2\pi\hbar^2} \int d^3\vec{r}' e^{-i\vec{k}'\cdot\vec{r}'} V(\vec{r}')\psi_{\vec{k}}(\vec{r}')$$
(13.84)

$$\psi_{\vec{k}}(\vec{r}) = \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) P_{\ell}(\cos\theta) R_{\ell}(r)$$
(13.85)

Using the relation

$$e^{-i\vec{k}\,'\cdot\vec{r}\,'} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-1)^{\ell} Y *_{\ell m} (\Omega_{\vec{k}\,\prime}) j_{\ell}(kr) Y_{\ell m}(\Omega_{\vec{r}\,\prime})$$
(13.86)

we get

$$f_{\vec{k}}(\theta,\varphi) = -\frac{2m}{\hbar^2} \int d^3\vec{r}' \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-1)^{\ell} Y *_{\ell m} (\Omega_{\vec{k}\,\prime}) j_{\ell}(kr') Y_{\ell m}(\Omega_{\vec{r}\,\prime}) V(\vec{r}\,') \\ \times \sum_{\ell'=0}^{\infty} i^{\ell'} (2\ell'+1) P_{\ell'}(\cos\theta) R_{\ell'}(r)$$
(13.87)

Now

$$\int d^{3}\vec{r}' \to \int_{0}^{2\pi} d\varphi_{\vec{r}\,'} \int_{-1}^{1} d(\cos\theta_{\vec{r}\,'}) \int_{0}^{\infty} r^{\,'2} dr\,' \tag{13.88}$$

and

 $\varphi_{\vec{r}\,'}$ integration $\rightarrow \delta_{m0}$ $\theta_{\vec{r}\,'}$ integration $\rightarrow \delta_{\ell\ell'}$

This implies (using $\theta_{\vec{k}},=\theta)$ that we get

$$f(\theta) = -\frac{2m}{\hbar^2} \sum_{\ell=0}^{\infty} (2\ell+1) P_{\ell}(\cos\theta) \int_{0}^{\infty} r^2 dr V(r) j_{\ell}(kr) R_{\ell}(r)$$
(13.89)

But we also have, in general, that

$$f(\theta) = \frac{1}{k} \sum_{\ell} (2\ell + 1) P_{\ell}(\cos \theta) e^{i\delta_{\ell}} \sin \delta_{\ell}$$
(13.90)

which then says that

$$e^{i\delta_{\ell}}\sin\delta_{\ell} = -\frac{2mk}{\hbar^2}\int_0^\infty r^2 dr V(r)j_{\ell}(kr)R_{\ell}(r)$$
(13.91)

If we suppose that the potential is weak for a particular partial wave, then we have very small scattering effects on $R_{\ell}(r)$. We then have

$$R_{\ell}(r) \approx j_{\ell}(kr) \tag{13.92}$$

and

$$e^{i\delta_{\ell}}\sin\delta_{\ell}\approx\delta_{\ell}\tag{13.93}$$

or

$$\delta_{\ell} = -\frac{2mk}{\hbar^2} \int_0^\infty r^2 dr V(r) j_{\ell}^2(kr)$$
(13.94)

This is the so-called *Born Approximation* for the phase shift δ_{ℓ} .

When the potential has a small effect on *all* partial waves we can derive another form of the Born approximation. In this case, we assume the scattered wave is small compared to the incident wave. This implies that

$$\psi_{\vec{k}}(\vec{r}) \to e^{i\vec{k}\cdot\vec{r}} \tag{13.95}$$

and

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int d^3\vec{r}' e^{-i(\vec{k}-\vec{k}')\bullet\vec{r}'} V(\vec{r}')$$
(13.96)

$$= -\frac{m}{2\pi\hbar^2} V_{\vec{k}\,'-\vec{k}} \tag{13.97}$$

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where

$$V_{\vec{k}\,'-\vec{k}}$$
 = Fourier transform of $V(\vec{r})$ (13.98)

Now we have elastic scattering $(|\vec{k}|=k=|\vec{k}\,'|) \text{which implies that}$

$$\vec{q} = \left| \vec{k} - \vec{k}' \right| \tag{13.99}$$

$$q^{2} = \left|\vec{k} - \vec{k}'\right|^{2} = k^{2} + k'^{2} - 2\vec{k} \cdot \vec{k}'$$
(13.100)

$$= 2k^2 - 2k^2 \cos \theta = 2k^2 (1 - \cos \theta)$$
(13.101)

$$= \left(2k\sin\frac{\theta}{2}\right)^2 \tag{13.102}$$

where θ is the scattering angle (angle between \vec{k} and \vec{k}') as shown in Figure 13.3 below.



Figure 13.3: Elastic Scattering Angles

When is the Born approximation valid?

For short range potentials, the wave function $\psi_{\vec{k}}(\vec{r})$ only contributes to the scattered wave at small distances. We can therefore use a small distance approximation for $\psi_{\vec{k}}(\vec{r})$

$$\psi_{\vec{k}}(\vec{r}) \approx e^{i\vec{k}\cdot\vec{r}} - \frac{m}{2\pi\hbar} \int d^3\vec{r}' \frac{e^{ikr'}}{r'} V(r') e^{i\vec{k}\cdot\vec{r}'} \approx e^{i\vec{k}\cdot\vec{r}}$$
(13.103)

only if

$$\left|\frac{m}{2\pi\hbar} \int d^{3}\vec{r}' \frac{e^{ikr'}}{r'} V(r') e^{i\vec{k}\cdot\vec{r}'}\right| = \left|\frac{m}{2\pi\hbar} \int r'^{2} dr' \frac{e^{ikr'}}{r'} V(r') \frac{\sin kr'}{kr'}\right| \ll 1$$

This corresponds to weak potentials and large k (or large energy).

13.1.6 A General Property of Phase Shifts

Let us assume the potential

$$V(r) = \begin{cases} 0 & r > b \\ v(r) & r \le b \end{cases}$$
(13.104)

The general results we will obtain are valid as long as $r^2 V(r) \to 0$ as $r \to \infty$.

For r > b, we have

$$\psi_{\ell}^{>}(r) = \frac{1}{2} \left[h_{\ell} * (kr) + e^{2i\delta_{\ell}} h_{\ell}(kr) \right]$$
(13.105)

For r < b, we must solve the Schrödinger equation with ? present. We assume that has been done and we obtained the solution $\psi_{\ell}^{<}(r)$.

At r = b, both the wave function and its derivative must be continuous, which implies that the logarithmic derivative is continuous

$$\alpha_{\ell} = \frac{\left(\frac{d\psi_{\ell}^{<}(r)}{dr}\right)_{r=b}}{\psi_{\ell}^{<}(b)} = \frac{\left(\frac{d\psi_{\ell}^{>}(r)}{dr}\right)_{r=b}}{\psi_{\ell}^{>}(b)}$$
(13.106)

or using our earlier expression for $\psi_{\ell}^{>}(r)$ we have

$$\alpha_{\ell} = \left(\frac{\frac{\partial}{\partial r} \left[h_{\ell} * (kr) + e^{2i\delta_{\ell}} h_{\ell}(kr)\right]}{h_{\ell} * (kr) + e^{2i\delta_{\ell}} h_{\ell}(kr)}\right)_{r=b}$$
(13.107)

Since $h_{\ell}(kr) = j_{\ell}(kr) + i\eta_{\ell}(kr)$, this gives

$$e^{2i\delta_{\ell}} - 1 = \left(\frac{2\left(\frac{dj_{\ell}(kr)}{dr} - \alpha_{\ell}j_{\ell}(kr)\right)}{\alpha_{\ell}h_{\ell}(kr) - \frac{dh_{\ell}(kr)}{dr}}\right)_{r=b} = \frac{2i}{\cot\delta_{\ell} - 1}$$
(13.108)

or

$$\cot \delta_{\ell} = \left(\frac{\frac{d\eta_{\ell}(kr)}{dr} - \alpha_{\ell}\eta_{\ell}(kr)}{\frac{dj_{\ell}(kr)}{dr} - \alpha_{\ell}j_{\ell}(kr)}\right)_{r=b}$$
(13.109)

13.1.7 Examples

Scattering from a Hard Sphere

In this case we have

$$V(r) = \begin{cases} 0 & r > b \\ \infty & r \le b \end{cases}$$
(13.110)

This is a repulsive potential. It implies that

$$\psi_{\ell}^{<}(r) = 0 \to \psi_{\ell}^{<}(b) = \psi_{\ell}^{>}(b) = 0$$
(13.111)

and

$$\alpha_{\ell} = \infty \tag{13.112}$$

This gives

$$\cot \delta_{\ell} = \frac{\eta_{\ell}(kb)}{j_{\ell}(kb)} \tag{13.113}$$

For $\ell=0$ we have

$$\cot \delta_0 = \frac{\eta_0(kb)}{j_0(kb)} = -\frac{\cos kb}{\sin kb} = -\cot kb$$
 (13.114)

 \mathbf{or}

$$\delta_0 = -kb \tag{13.115}$$

therefore, for a repulsive potential $\delta_0 < 0.$

What about δ_{ℓ} ? Consider low energy or small k. We then have for $kb \ll 1$,

$$\cot \delta_{\ell} = \frac{\eta_{\ell}(kb)}{j_{\ell}(kb)} \approx -\frac{\frac{(2\ell-1)!!}{(kb)^{\ell+1}}}{\frac{(kb)^{\ell}}{(2\ell+1)!!}} = -(kb)^{-2\ell-1}(2\ell-1)!!(2\ell+1)!!$$
(13.116)

where

$$(2\ell+1)!! = 1 \cdot 3 \cdot 5 \cdots (2\ell+1) \tag{13.117}$$

Therefore, we have

$$\sin \delta_{\ell} \approx (kb)^{2\ell+1} \tag{13.118}$$

Thus, we can neglect all terms where $\ell \neq 0$ in the low energy limit and write

$$f(\theta) = \frac{1}{k} P_0(\cos\theta) e^{i\delta_0} \sin\delta_0 = \frac{1}{k} e^{i\delta_0} \sin\delta_0 \qquad (13.119)$$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{\sin^2 \delta_0}{k^2} = b^2$$
(13.120)

$$\sigma = 4\pi \frac{\sin^2 \delta_0}{k^2} = 4\pi b^2 \tag{13.121}$$

These results for the hard sphere show that, for low energy, the total cross section is

 $4 \times ($ classical scattering cross section) (13.122)

due to quantum interference effects and the scattering is isotropic.

Scattering from a Potential Well

In this case

$$V(r) = \begin{cases} 0 & r > b \\ -V_0 & r \le b \end{cases}$$
(13.123)

The solution for positive energy inside the well is

$$\psi_{\ell}^{<}(r) = j_{\ell}(qr) \tag{13.124}$$

where

$$q = \sqrt{\frac{2m}{\hbar^2}(V_0 + E)}$$
(13.125)

Therefore, the boundary conditions at the well edge give

$$\alpha_{\ell} = \left(\frac{\frac{dj_{\ell}(qr)}{dr}}{j_{\ell}(qr)}\right)_{r=b}$$
(13.126)

Now

$$j_0(\rho) = \frac{\sin \rho}{\rho} , \quad j_1(\rho) = \frac{\sin \rho}{\rho^2} - \frac{\cos \rho}{\rho}$$
 (13.127)

$$\eta_0(\rho) = -\frac{\cos\rho}{\rho} \quad , \quad \eta_1(\rho) = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho} \tag{13.128}$$

Therefore,

$$\alpha_0 = q \cot qb - \frac{1}{b}$$
$$\alpha_0 b = qb \cot qb - 1$$

which gives

$$\cot \delta_0 = \left(\frac{\frac{d\eta_0(kr)}{dr} - \alpha_0 \eta_0(kr)}{\frac{dj_0(kr)}{dr} - \alpha_0 j_0(kr)}\right)_{r=b} = \frac{kb\sin kb + qb\cot qb\cos kb}{kb\cos kb - qb\cot qb\sin kb}$$
(13.129)

For $kb \ll 1$ we get

$$\cot \delta_0 = \frac{qb \cot qb}{kb(1 - qb \cot qb)} \tag{13.130}$$

 \mathbf{or}

$$\tan \delta_0 = -\frac{kb\alpha_0 b}{qb\cot qb} = -\frac{k\alpha_0 b^2}{1+\alpha_0 b}$$
(13.131)

In a similar manner, we can derive

$$\tan \delta_1 = \frac{(kb)^3}{3} \frac{1 - \alpha_1 b}{2 + \alpha_1 b} \tag{13.132}$$

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For low energy $(k \to 0)$ and a deep well $(V_0 \text{ large})$ we get

$$\sigma = 4\pi b^2 \left(1 - \frac{\tan qb}{qb}\right)^2 \tag{13.133}$$

This calculation fails if either

$$1 + \alpha_0 b = 0 \text{ or } 2 + \alpha_1 b = 0 \tag{13.134}$$

which corresponds to the $\ell=0$ or the $\ell=1$ partial wave being in resonance with the potential.

In general, this resonance condition is given by

$$\ell + 1 + \alpha_{\ell} b = 0 \tag{13.135}$$

which implies that

$$\cot \delta_{\ell} = 0 \to \tan \delta_{\ell} = \infty \to \delta_{\ell}(k) = \left(n + \frac{1}{2}\right)\pi$$
(13.136)

and thus the partial wave scattering cross section takes on its maximum value, namely,

$$\sigma_{\ell}(k) = \frac{4\pi(2\ell+1)}{k^2} \tag{13.137}$$

For other k values (off-resonance) we have

$$\delta_{\ell} \approx (kb)^{2\ell+1} \tag{13.138}$$

This says that the resonance is very sharp for large ℓ values.

We can understand this effect better by looking at other features. As we saw, for small k, $\cot \delta_{\ell}$ is very large since it is proportional to $k^{-2\ell-1}$. Therefore,

$$\sigma_{\ell} = \frac{4\pi}{k^2} (2\ell + 1) \sin^2 \delta_{\ell} = \frac{4\pi}{k^2} (2\ell + 1) \frac{1}{1 + \cot^2 \delta_{\ell}}$$
(13.139)

will be proportional to $k^{4\ell}.$ In this case, except for the s-wave $(\ell=0),\,\sigma_\ell$ will be small.

However, near a resonance energy E_r where

$$\ell + 1 + b\alpha_{\ell}(E_r) = 0 \tag{13.140}$$

 $\cot \delta_{\ell}$ goes to zero and σ_{ℓ} will be proportional to k^{-2} and this is quite large (an effect that is called resonance).

Near E_r we can make a Taylor expansion and write

$$\ell + 1 + b\alpha_{\ell}(E_r) \approx \ell + 1 + b\alpha_{\ell}(E_r) + (E - E_r)b\left(\frac{\partial\alpha_{\ell}}{\partial E}\right)_{E=E_r} + \dots$$
$$\approx (E - E_r)b\left(\frac{\partial\alpha_{\ell}}{\partial E}\right)_{E=E_r}$$
(13.141)

and

$$\ell - b\alpha_{\ell}(E_r) \approx 2\ell + 1 \tag{13.142}$$

After some algebra, these relations imply that

$$\cot \delta_{\ell} \approx -\frac{2(E - E_r)}{\Gamma_k} \tag{13.143}$$

where

$$\Gamma_k = -\frac{2k^{2\ell+1}b^{2\ell}}{\left[\left(2\ell-1\right)!!\right]^2 \left(\frac{\partial\alpha_\ell}{\partial E}\right)_{E=E_r}}$$
(13.144)

Now $\partial \alpha_{\ell} / \partial E < 0$, which implies that $\Gamma_k > 0$. Therefore, near resonance, the partial wave cross section σ_{ℓ} is

$$\sigma_{\ell} = \frac{4\pi \frac{\Gamma_k^2}{k^2}}{4(E - E_r)^2 + \Gamma_k^2}$$
(13.145)

When

$$E - E_r = \pm \frac{\Gamma_k}{2}$$
 (13.146)

the partial wave cross section is equal to one-half its maximum value. Therefore, $\Gamma = \Gamma_k(E_r)$ is the width of the resonance at half-maximum.

This functional form is called the *Breit-Wigner* formula for a scattering resonance. The curves are shown in Figure 13.4 below.


Figure 13.4: σ_ℓ versus E ; δ_ℓ versus E

which are standard resonance type curves.

13.1.8 Born Approximation Examples

Yukawa Potential

In this case

$$V(r) = a \frac{e^{-\mu r}}{r}$$
(13.147)

Although this potential is nonzero out to infinity, it is effectively short-range because it falls off exponentially. The *effective range* is usually given as $1/\mu$.

The Fourier transform of this potential is easily calculated to be

$$\tilde{V}(\vec{k} - \vec{k}') = \frac{4\pi a}{\left|\vec{k} - \vec{k}'\right|^2 + \mu^2}$$
(13.148)

where

$$\left|\vec{k} - \vec{k}'\right|^2 = \left(2k\sin\frac{\theta}{2}\right)^2$$
 (13.149)

This gives

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{(2\pi\hbar^2)^2} \left| \tilde{V}(\vec{k} - \vec{k}\,') \right|^2 = \frac{m^2}{(2\pi\hbar^2)^2} \left(\frac{4\pi a}{\left| \vec{k} - \vec{k}\,' \right|^2 + \mu^2} \right)^2$$
$$= \frac{a^2}{\left(4E_k \sin^2 \frac{\theta}{2} + \frac{\hbar^2 \mu^2}{2m} \right)^2}$$
(13.150)

By pure coincidence, if we let $\mu\to 0$ so that the Yukawa potential turns into the Coulomb potential we get the result

$$\frac{d\sigma}{d\Omega} = \frac{a^2}{16E_k^2 \sin^4 \frac{\theta}{2}} \tag{13.151}$$

which is the correct Rutherford cross section!

This is an accident and higher order terms will completely change this result. The higher order terms that we have neglected in the Born approximation cannot be ignored for a long-range potential like the Coulomb potential.

Later we will show how to handle Coulomb scattering correctly.

Scattering from Two Delta Functions

Here we have a free particle with momentum $p=\hbar k$ parallel to the z-axis scattering from the potential

$$V(\vec{r}) = v_0 \left[\delta(\vec{r} - \varepsilon \hat{z}) - \delta(\vec{r} + \varepsilon \hat{z}) \right]$$
(13.152)

Using $\vec{q} = \vec{k} - \vec{k}'$ as defined earlier, we have, in the Born approximation,

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int d^3\vec{r} \, V(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} = -\frac{mv_0}{2\pi\hbar^2} \left(e^{i\varepsilon\vec{q}\cdot\hat{z}} - e^{-i\varepsilon\vec{q}\cdot\hat{z}} \right)$$
$$= \frac{mv_0}{\pi\hbar^2} i\sin|q_z|\varepsilon$$
(13.153)

where

$$q_z = -q\sin\frac{\theta}{2} = -2k\sin^2\frac{\theta}{2} \tag{13.154}$$

is the projection of \vec{q} on the z-axis.

The scattering cross section is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{m^2 v_0^2}{\pi^2 \hbar^4} \sin^2 q_z \varepsilon$$
$$= \frac{m^2 v_0^2}{\pi^2 \hbar^4} \sin^2 \left(2\varepsilon k \sin^2 \frac{\theta}{2}\right)$$
(13.155)

which corresponds to the standard two-source interference pattern as expected.

Spin Dependent Potential

We now consider the scattering of a particle of mass m and momentum $p = \hbar k$ through an angle θ by the spin-dependent potential

$$V(\vec{r}) = e^{-\mu r^2} \left[A + B\vec{\sigma} \cdot \vec{r} \right]$$
(13.156)

where

$$\vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \tag{13.157}$$

We assume that the initial spin is along the incident direction and we sum over all final spins, which corresponds to measuring only the direction of the scattered particles and not their spins. Note that this potential violates parity.

We use the Born approximation. The Fourier transform of the potential function is given by

$$\tilde{V}(\vec{q}) = \int d^3 \vec{r} \, V(\vec{r}) e^{-i\vec{q}\cdot\vec{r}}$$
(13.158)

where

$$\vec{q} = \vec{k} - \vec{k}'$$
 (13.159)

We get

$$\widetilde{V}(\vec{q}) = \int d^{3}\vec{r} \, e^{-\mu r^{2}} \left[A + B\vec{\sigma} \cdot \vec{r} \right] e^{-i\vec{q}\cdot\vec{r}}
= \left(\frac{\pi}{\mu}\right)^{3/2} e^{-\frac{q^{2}}{4\mu}} \left[A + \frac{iB}{2\mu}\vec{\sigma} \cdot \vec{q} \right]
= \left(\frac{\pi}{\mu}\right)^{3/2} e^{-\frac{q^{2}}{4\mu}} \left[A + \frac{iB}{2\mu} \left[q_{+}\hat{\sigma}_{-} + q_{-}\hat{\sigma}_{+} + q_{z}\hat{\sigma}_{z} \right] \right]$$
(13.160)

where

$$q_{\pm} = q_x \pm iq_y \text{ and } \sigma_{\pm} = \frac{1}{2} \left(\sigma_x \pm i\sigma_y \right)$$
 (13.161)

Since the initial spin is oriented along \tilde{k} , which we choose to be in the z-direction, we also quantize the final spin along the same axis (use the same representation).

How do the different terms scatter spins?

- 1. The term A is spin-independent. This implies that the final spin state is the same as the initial spin state and the value of this term is A.
- 2. The term $Bq_z \hat{\sigma}_z$ is a diagonal operator in this representation. This implies that the final spin state is the same as the initial spin state and the value of this term is Bq_z . We only get the plus sign because we assumed spin up in the initial state.
- 3. The term $Bq_+\hat{\sigma}_-$ flips the spin from +z to -z. This implies the value is Bq_+ in a final state with the spin flipped(lowered).

4. The term $Bq_{-}\hat{\sigma}_{+}$ gives a zero contribution since the initial spin cannot be *raised*.

Therefore, if the final state is $|+z\rangle$ we get a contribution

$$A + \frac{i}{2\mu} Bq_z \tag{13.162}$$

and if the final state is $|-z\rangle$ we get a contribution

$$\frac{i}{2\mu}B(q_x + iq_y) \tag{13.163}$$

To get the total contribution to $f(\theta)$ we must square each separate term (these are not indistinguishable processes) and then sum over the final states. We get

$$\left|A + \frac{i}{2\mu}Bq_z\right|^2 + \left|\frac{i}{2\mu}B(q_x + iq_y)\right|^2 = A^2 + \frac{B^2q^2}{4\mu^2}$$
(13.164)

Therefore, the differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{\pi}{4\hbar v\mu^3} \int k'^2 dk' e^{-(\vec{k}-\vec{k}\,')^2/2\mu} \delta\left(\frac{\hbar^2}{2m} \left(k^2 - k\,'^2\right)\right) \left[A^2 + \frac{B^2(\vec{k}-\vec{k}\,')^2}{4\mu^2}\right] \\
= \frac{\pi^2 m^2}{4\hbar^4 \mu^3} e^{-k^2(1-\cos\theta)/2\mu} \left[A^2 + \frac{B^2 k^2(1-\cos\theta)}{2\mu^2}\right]$$
(13.165)

Scattering from Atomic Electrons

The atomic potential seen by an incoming electron can be represented by the function

$$V(r) = -Ze^2 \int \frac{\rho_T(\vec{r}\,')d^3\vec{r}\,'}{|\vec{r} - \vec{r}\,'|} \tag{13.166}$$

where

$$\rho_T(\vec{r}\,') = \rho_{nuclear}(\vec{r}\,') + \rho_{electronic}(\vec{r}\,') \\ = \delta(\vec{r}\,') - \rho(\vec{r}\,')$$

We then have

$$f(\theta) = \frac{mZe^2}{2\pi\hbar^2} \int \int \frac{\rho_T(\vec{r}\,')e^{i\vec{q}\cdot\vec{r}\,'}}{|\vec{r}-\vec{r}\,'|} d^3\vec{r}\,d^3\vec{r}\,'$$
$$= \frac{mZe^2}{2\pi\hbar^2} \int \rho_T(\vec{r}\,')e^{i\vec{q}\cdot\vec{r}\,'}d^3\vec{r}\,' \int \frac{e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}}{|\vec{r}-\vec{r}\,'|}d^3\vec{r}$$
(13.167)

In the last integral \vec{r}' is a constant. Therefore we can write

$$\int \frac{e^{i\vec{q}\cdot\vec{r}\cdot\vec{r}\,')}}{|\vec{r}-\vec{r}\,'|} d^{3}\vec{r} = \int \frac{e^{i\vec{q}\cdot\vec{x}}}{x} d^{3}\vec{x}$$

$$= \lim_{\alpha \to 0} \int_{0}^{2\pi} d\varphi \int_{0}^{\pi} \sin\theta d\theta \int_{0}^{\infty} e^{-\alpha x} e^{iqx\cos\theta} x dx$$

$$= 2\pi \lim_{\alpha \to 0} \int_{0}^{\infty} e^{-\alpha x} x dx \int_{\pi}^{0} d(\cos\theta) e^{iqx\cos\theta}$$

$$= 2\pi \lim_{\alpha \to 0} \int_{0}^{\infty} e^{-\alpha x} x dx \left[\frac{e^{iqx} - e^{-iqx}}{iqx} \right]$$

$$= \frac{4\pi}{q} \lim_{\alpha \to 0} \int_{0}^{\infty} e^{-\alpha x} \sin qx dx$$

$$= \frac{4\pi}{q} \lim_{\alpha \to 0} \frac{q}{q^{2} + \alpha^{2}} = \frac{4\pi}{q^{2}}$$
(13.168)

This trick of introducing the integrating factor $e^{-\alpha x}$ is a very useful procedure for evaluating this type of integral. We then have

$$f(\theta) = \frac{2mZe^2}{\hbar^2 q^2} \int \rho_T(\vec{r}\,') e^{i\vec{q}\cdot\vec{r}\,'} d^3\vec{r}\,'$$

$$= \frac{2mZe^2}{\hbar^2 q^2} \int \left[\delta(\vec{r}\,') - \rho(\vec{r}\,')\right] e^{i\vec{q}\cdot\vec{r}\,'} d^3\vec{r}\,'$$

$$= \frac{2mZe^2}{\hbar^2 q^2} \left[1 - F(q)\right]$$
(13.169)

where

$$F(q) = \int \rho(\vec{r}\,') e^{i\vec{q}\cdot\vec{r}\,'} d^3\vec{r}\,'$$
(13.170)

= the atomic scattering function energy of the nuclei

It is a measure of the amount of shielding of the nuclear charge by the electrons in the atom. It is the Fourier transform of the electron charge density.

13.2 Molecular Physics

13.2.1 General Properties of Molecules

Molecules are made up of nuclei and electrons. Since they break up into atoms if enough energy is supplied, we can regard them as bound states of atoms.

The determination of the electronic energy levels of molecules is significantly

more complicated than in atomic systems since the potential felt by the electrons does not exhibit many of the simplifying features of the atomic case.

On the other hand, nuclei are very massive compared to the electrons

$$\frac{m_e}{m_N} \approx 10^{-3} - 10^{-5} \tag{13.171}$$

and this can be used to simplify our work.

First, we must determine to what extent we need to take nuclear motion into account in our calculations. On the average, the nuclei move more slowly than the electron, have a small zero point energy and are well localized. We can picture the nuclei in a molecule as having classical equilibrium positions (minimum potential energy points) and that they oscillate slowly about these positions. In the meantime, the electrons are moving rapidly through the nuclear potentials. The electrons effectively see a static potential and the electronic wave functions can only be adiabatically changed by the slow nuclear vibrations. The nuclei have translational, vibrational and rotational motions that we must take into account.

What are the typical energies associated with these motions?

In a molecule of size a, the typical momentum is of order \hbar/a (due to the uncertainty principle). This implies that

$$E_{el}$$
 = typical electronic energy
 $\approx \frac{p^2}{2m} = \frac{\hbar^2}{2ma^2} \approx \text{ a few } eV$

To estimate the nuclear vibrational motion relative to the equilibrium positions, we assume a harmonic oscillator potential. The potential energy associated with each mode of vibration is then

$$\frac{1}{2}M\omega^2 R^2 \tag{13.172}$$

where

M = the nuclear mass R = amplitude of the oscillations ω = vibrational frequency

For R = a, the vibrational energy is approximately the same as the electronic energy. We see this as follows. We have

$$\frac{1}{2}M\omega^2 a^2 \approx \frac{\hbar^2}{2ma^2}$$
$$\omega \approx \left(\frac{m}{M}\right)^{1/2} \frac{\hbar^2}{ma^2}$$

Therefore, the total vibrational energy is

$$E_{vib} = \hbar\omega \approx \left(\frac{m}{M}\right)^{1/2} E_{el} \approx 0.01 - 0.1 \ eV \tag{13.173}$$

The rotational energy for an angular momentum $\ell \hbar$ is

$$E_{rot} \approx \frac{\hbar^2 \ell(\ell+1)}{2I} \approx \frac{\hbar^2}{Ma^2} = \frac{m}{M} E_{el}$$
(13.174)

Therefore, we have

$$E_{mol} = E_{el} + E_{vib} + E_{rot} \tag{13.175}$$

where the relative sizes are given by

$$E_{el}: E_{vib}: E_{rot} = 1: \left(\frac{m}{M}\right)^{1/2}: \frac{m}{M}$$
 (13.176)

In this model of a molecule we will use

$$\hat{H} = \hat{T}_e + \hat{T}_N + \hat{V}_{ee} + \hat{V}_{eN} + \hat{V}_{NN}$$
(13.177)

where

$$\hat{T}_e = \sum_{\substack{electrons}} \frac{\vec{p}_{op,i}^2}{2m} = \text{ kinetic energy of the electrons}$$

$$\hat{T}_N = \sum_{\substack{nuclei\\\alpha}} \frac{\vec{p}_{op,\alpha}^2}{2m} = \text{ kinetic energy of the nuclei}$$

$$\hat{V}_{ee} = \text{ repulsive electron - electron Coulomb interaction}$$

$$\hat{V}_{eN} = \text{ attractive electron - nucleus Coulomb interaction}$$

$$\hat{V}_{NN} = \text{ repulsive nucleus - nucleus Coulomb interaction}$$

Since the nuclear kinetic energy is proportional to 1/M, it is relatively small and we can treat it as a perturbation using the small perturbation parameter

$$\left(\frac{m}{M}\right)^{1/4} \tag{13.178}$$

Thus, we start the calculation by neglecting \hat{T}_N (neglecting the nuclear motion). In this approximation, the nuclear coordinates \vec{R} are fixed, which implies that they are no longer dynamical variables (observables) but only parameters. The Schrodinger equation is then

$$(\hat{T}_e + \hat{V}_{ee} + \hat{V}_{eN})\psi_n(\vec{r}, \vec{R}) = (\varepsilon_n(\vec{R}) - \hat{V}_{NN}(\vec{R}))\psi_n(\vec{r}, \vec{R})$$
(13.179)

$$= E_{el}(\vec{R})\psi_n(\vec{r},\vec{R})$$
(13.180)

Here we have defined

$$\varepsilon_n(\vec{R}) = \text{NN interaction energy} + \text{the electronic energy eigenvalue}$$

= $E_{el}(\vec{R}) + \hat{V}_{NN}(\vec{R})$
 $\psi_n(\vec{r}, \vec{R}) = \text{wave function of the electrons (remember $\vec{R} \text{ is fixed})$
 $\vec{r} \text{ represents the coordinates of all the electrons}$$

Now the wave function for the whole molecule satisfies the Schrodinger equation

$$(\hat{T}_e + \hat{T}_N + \hat{V}_{ee} + \hat{V}_{eN} + \hat{V}_{NN})\psi(\vec{r}, \vec{R}) = E\psi(\vec{r}, \vec{R})$$
(13.181)

The solutions $\psi_n(\vec{r}, \vec{R})$ form a complete set of basis functions. Therefore we can write

$$\psi(\vec{r}, \vec{R}) = \sum_{n} \phi_n(\vec{R}) \psi_n(\vec{r}, \vec{R})$$
 (13.182)

where the $\varphi_n(\vec{R})$ = expansion coefficients. Our task is to find the $\varphi_n(\vec{R})$.

Substituting we get

$$\begin{split} &\sum_{m} \left(\hat{T}_{e} + \hat{T}_{N} + \hat{V}_{ee} + \hat{V}_{eN} + \hat{V}_{NN} \right) \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) = E \sum_{m} \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) \\ &\sum_{m} \left(\hat{T}_{N} + \hat{V}_{NN} \right) \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) + \sum_{m} \left(\hat{T}_{e} + \hat{V}_{ee} + \hat{V}_{eN} \right) \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) \\ &= E \sum_{m} \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) \\ &\sum_{m} \left(\hat{T}_{N} + \hat{V}_{NN} \right) \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) + \sum_{m} \left(\varepsilon_{m}(\vec{R}) - \hat{V}_{NN}(\vec{R}) \right) \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) \\ &= E \sum_{m} \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) \\ &\sum_{m} \left(\hat{T}_{N} + \varepsilon_{m}(\vec{R}) \right) \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) = E \sum_{m} \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) \end{split}$$

If we multiply on the left by $\psi_n^*(\vec{r}, \vec{R})$ and integrate over all electron positions using the orthonormality of the $\psi_m(\vec{r}, \vec{R})$ we get

$$\sum_{m} \int d^{3}r \psi_{n}^{*}(\vec{r},\vec{R})(\hat{T}_{N} + \varepsilon_{m}(\vec{R}))\phi_{m}(\vec{R})\psi_{m}(\vec{r},\vec{R})$$

$$= E \sum_{m} \phi_{m}(\vec{R}) \int d^{3}r \psi_{n}^{*}(\vec{r},\vec{R})\psi_{m}(\vec{r},\vec{R})$$

$$\sum_{m} \int d^{3}r \psi_{n}^{*}(\vec{r},\vec{R})\hat{T}_{N}\phi_{m}(\vec{R})\psi_{m}(\vec{r},\vec{R}) + \sum_{m} \varepsilon_{m}(\vec{R})\phi_{m}(\vec{R})\delta_{nm}$$

$$= E \sum_{m} \phi_{m}(\vec{R})\delta_{nm}$$

$$\sum_{m} \int d^{3}r \psi_{n}^{*}(\vec{r},\vec{R})\hat{T}_{N}\phi_{m}(\vec{R})\psi_{m}(\vec{r},\vec{R}) + \varepsilon_{n}(\vec{R})\phi_{n}(\vec{R})$$

$$= E\phi_{n}(\vec{R})$$

Now \hat{T}_N contains 2^{nd} derivatives with respect to the \vec{R} and thus it acts on both functions $\phi_m(\vec{R})$ and $\psi_m(\vec{r}, \vec{R})$. Using

$$\nabla^{2}(\phi\psi) = (\nabla^{2}\phi)\psi + 2\nabla\phi \cdot \nabla\psi + \phi(\nabla^{2}\psi)$$
(13.183)

we have

$$\begin{split} \sum_{m} \int d^{3}r \psi_{n}^{*}(\vec{r},\vec{R}) \sum_{\alpha} \frac{\hbar^{2}}{2M_{\alpha}} \nabla_{\vec{R}_{\alpha}}^{2} \phi_{m}(\vec{R}) \psi_{m}(\vec{r},\vec{R}) + \varepsilon_{n}(\vec{R}) \phi_{n}(\vec{R}) \\ &= E \phi_{n}(\vec{R}) \\ \sum_{\alpha} \frac{\hbar^{2}}{2M_{\alpha}} \sum_{m} \int d^{3}r \psi_{n}^{*}(\vec{r},\vec{R}) [\psi_{m}(\vec{r},\vec{R}) \nabla^{2} \phi_{m}(\vec{R}) \\ &+ 2 \nabla \phi_{m}(\vec{R}) \cdot \nabla \psi_{m}(\vec{r},\vec{R}) + \phi_{m}(\vec{R}) \nabla^{2} \psi_{m}(\vec{r},\vec{R})] + \varepsilon_{n}(\vec{R}) \phi_{n}(\vec{R}) = E \phi_{n}(\vec{R}) \\ \sum_{\alpha} \frac{\hbar^{2}}{2M_{\alpha}} \sum_{m} \nabla^{2} \phi_{m}(\vec{R}) \int d^{3}r \psi_{n}^{*}(\vec{r},\vec{R}) \psi_{m}(\vec{r},\vec{R}) \\ &+ \sum_{\alpha} \frac{\hbar^{2}}{2M_{\alpha}} \sum_{m} \int d^{3}r \psi_{n}^{*}(\vec{r},\vec{R}) [2 \nabla \phi_{m}(\vec{R}) \cdot \nabla \psi_{m}(\vec{r},\vec{R}) \\ &+ \phi_{m}(\vec{R}) \nabla^{2} \psi_{m}(\vec{r},\vec{R})] + \varepsilon_{n}(\vec{R}) \phi_{n}(\vec{R}) = E \phi_{n}(\vec{R}) \end{split}$$

$$\sum_{\alpha} \frac{\hbar^2}{2M_{\alpha}} \sum_{m} \nabla^2 \phi_m(\vec{R}) \delta_{nm} + \sum_{\alpha} \frac{\hbar^2}{2M_{\alpha}} \sum_{m} \int d^3 r \psi_n^*(\vec{r}, \vec{R}) [2\nabla \phi_m(\vec{R}) \cdot \nabla \psi_m(\vec{r}, \vec{R}) + \phi_m(\vec{R}) \nabla^2 \psi_m(\vec{r}, \vec{R})] + \varepsilon_n(\vec{R}) \phi_n(\vec{R}) = E \phi_n(\vec{R})$$

$$\begin{split} \sum_{\alpha} \frac{\hbar^2}{2M_{\alpha}} \nabla_{\vec{R}_{\alpha}}^2 \phi_n(\vec{R}) \\ &+ \sum_{\alpha} \frac{\hbar^2}{2M_{\alpha}} \sum_m \int d^3 r \psi_n^*(\vec{r}, \vec{R}) [2\nabla \phi_m(\vec{R}) \cdot \nabla \psi_m(\vec{r}, \vec{R}) + \phi_m(\vec{R}) \nabla^2 \psi_m(\vec{r}, \vec{R})] \\ &+ \varepsilon_n(\vec{R}) \phi_n(\vec{R}) = E \phi_n(\vec{R}) \end{split}$$

 $\hat{T}_N \phi_n(\vec{R})$

$$+ \sum_{\alpha} \frac{\hbar^2}{2M_{\alpha}} \sum_{m} \int d^3 r \psi_n^*(\vec{r}, \vec{R}) [2\nabla \phi_m(\vec{R}) \cdot \nabla \psi_m(\vec{r}, \vec{R}) + \phi_m(\vec{R}) \nabla^2 \psi_m(\vec{r}, \vec{R})]$$
$$+ \varepsilon_n(\vec{R}) \phi_n(\vec{R}) = E \phi_n(\vec{R})$$

 or

$$(\hat{T}_N + \varepsilon_n(\vec{R}))\phi_n(\vec{R}) = E\phi_n(\vec{R}) - \sum_m A_{nm}\phi_m(\vec{R})$$
(13.184)

where

$$\begin{aligned} A_{nm}\phi_m(\vec{R}) \\ &= -\sum_{\alpha} \frac{\hbar^2}{2M_{\alpha}} \int d^3r \psi_n^*(\vec{r},\vec{R}) [2\nabla_{\vec{R}_{\alpha}}\phi_m(\vec{R}) \cdot \nabla_{\vec{R}_{\alpha}}\psi_m(\vec{r},\vec{R}) + \phi_m(\vec{R})\nabla_{\vec{R}_{\alpha}}^2\psi_m(\vec{r},\vec{R})] \end{aligned}$$

The A_{nm} term mixes different n and m, which corresponds to different electronic wave functions in $\psi(\vec{r}, \vec{R})$.

How large is this term? The term

$$-\frac{\hbar^2}{2M_{\alpha}} \nabla^2_{\vec{R}_{\alpha}} \psi_n(\vec{R}) \approx -\left(\frac{m}{M}\right) \frac{\hbar^2}{2m} \nabla^2_{\vec{r}} \psi_n(\vec{r})$$
$$\rightarrow \left(\frac{m}{M}\right) \times \text{ electron kinetic energy}$$

Since this is very much less than the spacing between different n levels, it implies that we will have negligible mixing of different n states. Now

$$\phi_m(R) \approx \text{ harmonic oscillator wave function}$$
$$\approx e^{-\frac{(\vec{R} - \vec{R}_0)^2 M \omega}{2\hbar}}$$
$$\nabla_{\vec{R}} \phi_m(\vec{R}) \approx \left| \vec{R} - \vec{R}_0 \right| \frac{M \omega}{\hbar} \phi_m(\vec{R}) \approx \delta \frac{M \omega}{\hbar} \phi_m(\vec{R})$$

where $\delta \approx$ typical nuclear displacement from equilibrium. But

$$\frac{1}{2}M\omega^2\delta^2 \approx \hbar\omega \tag{13.185}$$

This implies the first term in A_{nm} is of order

$$\hbar\omega \approx \left(\frac{m}{M}\right)^{1/2} \times \text{ spacing between } n|text-levels$$
 (13.186)

Therefore we can neglect all of the A_{nm} terms. We thus have

$$(\hat{T}_N + \varepsilon_n(\vec{R}))\phi_n(\vec{R}) = E\phi_n(\vec{R})$$
(13.187)

This is a simple Schrödinger equation for the $\phi_n(\vec{R})$, which are the expansion coefficients and therefore we can write down $\psi(\vec{r}, \vec{R})$ once we know the $\psi_n(\vec{r}, \vec{R})$.

The term $\varepsilon_n(\vec{R})$ is the total electron energy and it has become the effective potential energy for the nuclear motion in this approximation.

The effect of the electrons is to couple together the nuclei with *rubber bands* whose force constants depend on the electronic state. Thus, for each $\psi_n(\vec{r}, \vec{R})$, we have an $\varepsilon_n(\vec{R})$ which implies a $\phi_n(\vec{R})$. To lowest order in

$$\left(\frac{m}{M}\right)^{1/2} \tag{13.188}$$

we have no mixing of different n-levels.

We can therefore write the stationary states of the molecule as

$$\psi_n^{(\alpha)}(\vec{r}, \vec{R}) = \phi_{\alpha n}(\vec{R})\psi_n(\vec{r}, \vec{R})$$
 (13.189)

with an energy $E_{\alpha n}$ of the molecule, where α labels different solutions to

$$(\hat{T}_N + \varepsilon_n(\vec{R}))\phi_{\alpha n}(\vec{R}) = E_{\alpha n}\phi_{\alpha n}(\vec{R})$$
(13.190)

This approximation is the so-called *Born-Oppenheimer* approximation.

13.2.2 The Born-Oppenheimer approximation: A toy version

Before proceeding with more complicated examples, we illustrate the Born-Oppenheimer approximation, which, as we have described, is central to the physics and chemistry of molecules and solids, by a one-dimensional toy model that is easily solved.

Review of method and motivation

As we said earlier, molecules and solids are describable in terms of the motion of the electrons and nuclei of the constituent atoms. Although this description is immensely complicated, the fact that nuclei are much heavier than electrons makes it possible to adopt an approach in which the nuclei, in the lowest order of approximation, are taken to be at rest, and their motion is considered subsequently in higher orders.

This toy model is a simplification that makes the solution more transparent and analytically tractable.

Review of prior derivation

For molecules the underlying Hamiltonian of the system is

$$H = \sum_{i} \frac{\mathbf{p}_{i}^{2}}{2m} - \sum_{\mu,i} \frac{Z_{\mu}e^{2}}{|\mathbf{R}_{\mu} - \mathbf{r}_{i}|} + \sum_{i>j} \frac{e^{2}}{|\mathbf{r}_{i} - \mathbf{r}_{j}|} + \sum_{\mu} \frac{\mathbf{P}_{\mu}^{2}}{2M_{\mu}} + \sum_{\mu>\nu} \frac{Z_{\mu}Z_{\nu}e^{2}}{|\mathbf{R}_{\mu} - \mathbf{R}_{\nu}|}$$
(13.191)

where the upper-case letters, **R** and **P**, denote the position and momentum operators of the nuclei which are indexed by Greek letters. Lower-case letters, **r** and **p**, and Latin subscripts are reserved for the electrons; *m* is the mass of an electron, M_{μ} is the mass of the μ^{th} nucleus, -e is the electron charge, and $+Z_{\mu}e$ is the charge on the μ^{th} nucleus. The Schrödinger equation for the stationary states of the molecule is

$$\begin{bmatrix}
\frac{\hbar^2}{2m} \sum_{i} \nabla_i^2 - \sum_{\mu,i} \frac{Z_{\mu} e^2}{|\mathbf{R}_{\mu} - \mathbf{r}_i|} + \sum_{i>j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \\
+ \sum_{\mu} \frac{\hbar^2}{2M_{\mu}} \nabla_{\mu}^2 + \sum_{\mu>\nu} \frac{Z_{\mu} Z_{\nu} e^2}{|\mathbf{R}_{\mu} - \mathbf{R}_{\nu}|} \end{bmatrix} \psi(\{\mathbf{r}\}, \{\mathbf{R}\}) = E\psi(\{\mathbf{r}\}, \{\mathbf{R}\}) \quad (13.192)$$

The first step in the Born-Oppenheimer approach consists in asserting that the kinetic energy term associated with the heavy particles may be neglected in the lowest approximation and their coordinates treated as parameters (and not as dynamical variables). We write the full Hamiltonian as $H = H_0 + \hat{T}_R$ where H_0 is the electronic Hamiltonian in which the nuclear coordinates appear as parameters. The eigenfunctions and eigenvalues of H_0 describe the electrons for fixed values of the coordinates of the nuclei:

$$H_0\phi_n(\{\mathbf{r}\};\{\mathbf{R}\}) = \epsilon_n(\{\mathbf{R}\})\phi_n(\{\mathbf{r}\};\{\mathbf{R}\})$$
(13.193)

We write $\{\mathbf{R}\}$ after a semicolon to indicate that $\{\mathbf{R}\}$ appear only as parameters. The eigenvalues $\epsilon_n(\{\mathbf{R}\})$ depend on the particular values of $\{\mathbf{R}\}$ of the nuclei and yield energy surfaces that are labeled by n, the electronic quantum numbers. Because the states $\phi_n(\{\mathbf{r}\}; \{\mathbf{R}\})$ are a complete set of orthonormal vectors, we can use them as a basis to write the full wave function as

$$\psi(\{\mathbf{r}\};\{\mathbf{R}\}) = \sum_{n} \chi_n(\{\mathbf{R}\})\phi_n(\{\mathbf{r}\};\{\mathbf{R}\})$$
(13.194)

with the understanding that the summation includes integra- tion over continuum states. If we substitute the expansion (13.194) into Eq. (13.192) and integrate over the electronic coordinates, we obtain a set of coupled equations describing the dynamics of the heavy nuclei, namely,

$$\begin{bmatrix}
-\sum_{\mu} \frac{\hbar^2}{2M_{\mu}} \nabla_{\mu}^2 + \epsilon_n(\{\mathbf{R}\}) - E \end{bmatrix} \chi_n(\{\mathbf{R}\}) \\
\sum_{\mu,m} \begin{bmatrix} \int \phi_n^*(\{\mathbf{r}\}; \{\mathbf{R}\}) \nabla_{\mu} \phi_m(\{\mathbf{r}\}; \{\mathbf{R}\}) \Pi_i d^3 \mathbf{r}_i \end{bmatrix} \\
\times \nabla_{\mu} \chi_m(\{\mathbf{R}\}) + \sum_{\mu,m} \begin{bmatrix} \int \phi_n^*(\{\mathbf{r}\}; \{\mathbf{R}\}) \\
\times \left(-\frac{\hbar^2}{2M_{\mu}} \nabla_{\mu}^2\right) \phi_m(\{\mathbf{r}\}; \{\mathbf{R}\}) \Pi_i d^3 \mathbf{r}_i \}) \end{bmatrix} \chi_m(\{\mathbf{R}$$
(13.195)

where $m \neq n$. The terms on the left-hand side describe the motion driven by the kinetic energy operator of the nuclei on a given electronic energy surface $\epsilon_n(\{\mathbf{R}\})$, whereas those on the right-hand side represent *jumps* from one energy surface to another $(n \rightarrow m)$ resulting in the coupling of the different electronic states.

Equation (13.195) represents a formidable set of coupled equations which involve no approximations. The Born-Oppenheimer approximation asserts that the terms on the right-hand side of Eq. (13.195) may be neglected. Hence, the equation for the heavy nuclei, which are confined to the nth electronic energy surface, becomes

$$\left[-\sum_{\mu}\frac{\hbar^2}{2M_{\mu}}\nabla^2_{\mu} + \epsilon_n(\{\mathbf{R}\}) - E\right]\chi_n(\{\mathbf{R}\}) = 0$$
(13.196)

Equation (13.196) is tantamount to the statement that the different electronic energy surfaces $\epsilon_n(\{\mathbf{R}\})$ do not intersect or come close to each other in the relevant region of parameter space and are sufficiently distant in energy so that they are not appreciably connected by the kinetic motion of the nuclei. That is, the time scale of nuclear motions is slow compared to the movements of the light electrons or, in other words, the amplitudes of the nuclear motion are negligible in comparison with the equilibrium internuclear distances. Once this simplification is made, the motion of the nuclei can be further investigated via Eq. (13.196) to obtain the vibrations about the minima of $\epsilon_n(\{\mathbf{R}\})$ and the rotations of the molecules.

Real molecular systems are very complicated except for simple examples such as the hydrogen molecular ion H_2^+ (see below). To illustrate the basic ideas in a simple setting, we discuss a one-dimensional model of the actual physical system.

The Toy Model

Imagine a system of two particles: one light (of mass m) with coordinate x and the other heavy (mass M) located at X. The particles are confined between two impenetrable walls a distance L apart, that is, $-L/2 \leq x, X \leq L/2$. We assume that these two particles interact with each other via an attractive Dirac delta function interaction of strength λ . The Hamiltonian of the system within the allowed range is thus

$$H = \frac{p^2}{2m} + \frac{P^2}{2M} - \lambda \delta(x - X)$$
(13.197)

where p and P are the momenta of the two particles. The stationary states are given by

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2} - \lambda\delta(x-X)\right]\psi(x,X) = E\psi(x,X)$$
(13.198)

We follow the Born-Oppenheimer approach and first solve for the energy levels of the light particle, $E_n(X)$, treating X as a parameter, that is,

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \lambda\delta(x-X)\right]\phi(x;X) = \epsilon\phi(x;X)$$
(13.199)

or

$$\left[\frac{d^2}{dx^2} + k^2\right]\phi(x;X) = -\lambda\delta(x-X)\phi(x;X)$$
(13.200)

where $k^2 \equiv 2m\epsilon/\hbar^2$ and $\lambda \equiv 2m\lambda/\hbar^2$. The wave function ϕ satisfies the boundary conditions, $\phi(x = \pm L/2, X) = 0$. Thus for x < X the solution is $A \sin k(x + L/2)$ while for x > X we must have $B \sin k(L/2 - x)$, where A and B are constants. The continuity of the wave function at x = X implies that

$$A\sin k\left(\frac{L}{2}+X\right) = B\sin k\left(\frac{L}{2}-X\right) \tag{13.201}$$

The first derivative of the wave function must be discontinuous so as to yield the delta function in Eq. (13.200), whose integral between $x = X^-$ and $x = X^+$ yields the condition $\phi'(x = X^+); X) - \phi'(x = X^-; X) = -\lambda \phi(x = X; X)$, or

$$-Bk\cos k\left(\frac{L}{2}-X\right) - Ak\cos k\left(\frac{L}{2}+X\right) = -\lambda A\sin k\left(\frac{L}{2}+X\right)$$
(13.202)

If we eliminate A and B from Eqs. (13.201) and (13.202), we find the eigenvalue condition for k (and hence $\epsilon = \hbar^2 k^2/2m$):

$$k\sin kL = \lambda\sin k\left(\frac{L}{2} + X\right)\sin k\left(\frac{L}{2} - X\right)$$
(13.203)

For a given λ and L, Eq. (13.203) is to be solved for k as a function of X to determine the energy surfaces (here *curves* as there is only one parameter X). We observe that for $X = \pm L/2$ the right-hand side of the eigenvalue condition, Eq.(13.203) vanishes and $\sin kL = 0$ has the solutions $k = n\pi/L$ and $\epsilon_n = \hbar^2 n^2 \pi^2/(2mL)^2$. In other words, the infinite repulsion at the walls makes the wave function of the light particle (and hence the probability of finding it) zero at $X = \pm L/2$, and hence it must disregard the presence of the heavy particle if the latter is located at either of these two places.

As we consider values of X away from $X = \pm L/2$, the value of k must be determined by solving Eq. (13.203) and would be less than or equal to $n\pi/L$ because of the attractive delta function potential. Furthermore, the energy curves belonging to different n cannot cross each other as X varies, because such one-dimensional systems cannot possess any degeneracy. Thus we may use the integer n to label the states corresponding to the motion of the light particles analogous to the set of quantum numbers used to designate the state of an electron in a molecule. Moreover, the eigenvalue condition in Eq. (13.203) is symmetric under the transformation $X \to -X$, and hence it suffices to examine the range of X between 0 to L/2.

In the above discussion we have tacitly assumed that $\epsilon > 0$ by taking trigonometric functions as the solutions of Eq. (13.200), which generally holds except for the lowest state (and that too only if λ is large enough). The condition for crossover from positive to negative ϵ is easily derived by noting that if ϵ becomes negative, it must pass through zero and hence we can consider the eigenvalue condition, Eq. (13.203), for small k to obtain the critical potential strength

$$\lambda = \lambda_c = \frac{L}{\frac{L^2}{4} - X^2} \tag{13.204}$$

If $\lambda > \lambda_c$ for a range of X values, we must use the hyperbolic solutions of the Schrodinger equation with $|\epsilon| = -\epsilon = \hbar^2 k^2/2m$, and the eigenvalue condition becomes

$$k\sinh kL = \lambda \sinh k \left(\frac{L}{2} + X\right) \sinh k \left(\frac{L}{2} - X\right)$$
(13.205)

Equation (13.205) admits only one solution for the corresponding k. The reason is physically transparent. Note that for $L \to \infty, \lambda_c \to 0$, which means that as the walls recede to infinity, the attractive delta function potential no matter how weak will have a solution with a negative energy eigenvalue (as can be seen by solving the delta function potential without walls). Hence, in the presence of the repulsive walls, this energy eigenvalue can be negative provided the walls are not too close and the potential not too weak.

The nature of the energy surfaces is easily revealed by analyzing k as a function of X as given by Eq. (13.203). The location of the extrema is obtainable from

$$\frac{dk}{dX} = \frac{-\lambda k \sin 2kX}{\sin kL + kL \cos kL + \lambda X \sin 2kX - \frac{\lambda L}{2} \sin kL} = 0$$
(13.206)

which yields $2kX = \pm N\pi$ (N = 0, 1, 2, ...). For the lowest positive energy state, n = 1, there will be only one extremum at X = 0 (corresponding to N = 0), and this energy must be a minimum as can be seen from the following argument. At $X = \pm L/2$ we have $k = \pi/L$, and as we move the heavy particle away from the wall, the energy and hence k must de- crease because of the attractive nature of the interaction. Thus for the n = 1 energy surface, X = 0 is a minimum. For the first excited electronic state, n = 2, we have three extrema at N = 0 and ± 1 . The point X = 0 (corresponding to N = 0) is a maximum, because the vanishing of the wave function at x = 0 with X = 0 (the wave function is an odd function) implies that the derivative is continuous and hence the energy corresponds to $k = 2\pi/L$ (as if the light particle disregards the presence of the heavy one). As the heavy particle moves away from X = 0, the energy must decrease due to the onset of the nonzero attraction. Thus the n = 2 energy surface gives rise to a double well. Similarly, it is easy to see that for the second excited electronic state, there are three minima at X = 0 and $X = \pm \pi/k$ and two maxima at $X = \pm \pi/2k.$

The wave functions for the ground and first excited electronic states are shown in Fig. 13.5

with the heavy particle located at X = L/4 and the strength of the delta function corresponding to $\lambda = 2/L$. We have taken L = 1. Attention is drawn to the discontinuity in the derivative of the wave function of the light particle at the location of the heavy particle (indicated by the arrow). The shape and symmetry of the wave functions are clearly affected by the location of the heavy particle and the strength of the delta function interaction.

Now that we have solved for the motion of the light particle with the heavy particle at X, we may, in the spirit of the Born-Oppenheimer approach, turn our attention to the slower vibrational motion of the heavy particle governed by the potential surfaces, $\epsilon_n(X)$, obtained from $\epsilon = \hbar^2 k^2/2m$, where k are solutions (labeled by the quantum number n) of Eq. (13.203). The vibrational energies may be determined numerically given the values of the relevant parameters (m, M, λ, L) . However, these energies can be estimated via the harmonic



Figure 13.5: Wave function for the light particle when the heavy one is located at X=L/4 taking $\lambda=2/L$

approximation by using the curvature of the potential at the minima

$$\frac{d^2\epsilon(X)}{dX^2} = \frac{\hbar^2 k^2}{2m} \left[-\frac{4\lambda k \cos 2kX}{C} + \frac{2\lambda^2 \sin 2kX(\sin 2kX + 2kX \cos 2kX)}{C^2} \right]$$
(13.207)

where the dimensionless quantity $C = kL \cos kL + \lambda X \sin 2kX + (1 - \lambda L/2) \sin kL$.

For convenience we choose the value $\lambda = 2/L$. For the ground state electronic configuration, the minimum of the potential $\epsilon(X) = \epsilon_1(X)$ is at X = 0 and the corresponding solution of Eq. (13.203) yields kL = 2.33 (and $\cos kL = -0.69$). At the minimum of the potential, the curvature is

$$\frac{d^2\epsilon(X)}{dX^2} = -\frac{4\hbar^2k^2}{mL^2\cos kL} \tag{13.208}$$

leading to the classical angular frequency

$$\omega = \sqrt{\frac{d^2 \epsilon(X)/dX^2}{M}} \tag{13.209}$$

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The ensuing spectra is a ladder with spacing $\hbar\omega$, and accordingly, the vibrational energy levels are approximately given by

$$\hbar\omega\left(\nu + \frac{1}{2}\right) = \frac{\hbar^2}{2mL^2}\sqrt{\frac{16m}{M}\frac{k^2L^2}{|\cos kL|}}\left(\nu + \frac{1}{2}\right)$$
(13.210)

where ν is the vibrational quantum number and takes integer values 0, 1, 2, ...

To make contact between the toy model and the realistic situation of molecules, we take L to be of the order of chemical bond lengths $(L \sim 1)$ and m and M to be the masses of the electron and the proton, respectively, $m = 10^{-30} kg$ and $M \sim 2000m$. The separations between the electronic levels are thus of the order of $\Delta \sim (\hbar^2/mL^2) \sim 6 eV$, and the vibrational level spacings are $\hbar\omega \sim \hbar^2/(mL^2)\sqrt{m/M} \sim 0.1 \, eV$.

In Figures. 13.6 and 13.7 the potential energy surfaces (in units of $\hbar^2/2mL^2$) of the ground and first excited electronic states are plotted against X (in units of L) for $\lambda = 2.0/L$.



Figure 13.6: Potential energy surface (in units of $\hbar^2/2mL^2$ of the ground electronic state (n = 1) plotted against X (in units of L) for $\lambda = 2.0/L$. We have shown the vibrational bound states for $M \sim 2000m$. Note the decreasing separation between the adjacent levels, particularly for higher excitations, which reflects the anharmonicity of the potential surface.



Figure 13.7: Potential energy surface of the first excited (n = 2) electronic state for the same parameters as in Figure 13.6. Each energy level is almost doubly degenerate which undergoes splitting due to tunneling between the wells through the potential barrier. Splitting, though not discernible for the lower states, is clearly evident for the highest vibrational pair of levels.

It can be seen that for M = 2000m, the energy separation of the lower vibrational levels is almost 0.26(in units of $\hbar^2/2mL^2$). Thus a quadratic fit to the potential surface of the electronic ground state is very good at least for the lower vibrational levels (the agreement is within 5%). Similarly, for the first excited electronic state (n = 2), we have a double well potential surface and the curvature at the minima both correspond to an energy separation of 0.56. Indeed the results of a numerical calculation reveal that the almost equidistant vibrational level structure is obtained for the low lying levels, but the energy gaps reduce with increasing vibrational energy as the anharmonicity of the potential surface becomes important. Another feature of the first excited state, which is typical of a double well potential, is the occurrence of a doublet due to a degenerate pair of levels corresponding to each well split due to their coupling from tunneling through the barrier. This split- ting is too small to be seen in Figure 13.7 for the lower vibrational excitation and barely discernible in the next to highest vibrational level (shown by the thickening of this line in the diagram) and is clearly evident in the highest vibrational doublet. Hence, we see that many features of molecular systems apart from the methodology of the Born-Oppenheimer adiabatic approximation find a simple illustration in the toy model that we have discussed.

13.2.3 Examples

Hydrogen Molecular Ion (H_2^+)

In the ionized H_2 molecule, a single electron moves in the attractive potential of two protons A and B as shown in Figure 13.8 below.



Figure 13.8: Hydrogen Molecular Ion Configuration

The Hamiltonian, in the Born-Oppenheimer approximation, is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{\left|\vec{r} - \vec{R}_A\right|} - \frac{e^2}{\left|\vec{r} - \vec{R}_B\right|} + \frac{e^2}{\left|\vec{R}_A - \vec{R}_B\right|}$$
(13.211)

We will solve the problem using the variational method.

As a trial function we use a linear combination of hydrogen atom 1s states for separate protons:

$$\psi_{\pm} = C_{\pm} \left[\psi_A(\vec{r}) \pm \psi_B(\vec{r}) \right]$$
(13.212)

where we have chosen the symmetric and antisymmetric combinations only because the potential is symmetric about the midpoint of the molecule

$$\frac{\vec{R}_A + \vec{R}_B}{2} \tag{13.213}$$

The wave functions are

$$\psi_A(\vec{r}) = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{|\vec{r}-\vec{R}_A|}{a}} \text{ and } \psi_B(\vec{r}) = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{|\vec{r}-\vec{R}_B|}{a}}$$
(13.214)

The C_{\pm} are normalization factors given by

$$1 = \int d^3r |\psi_{\pm}(\vec{r})|^2 = C_{\pm}^2 \int d^3r |\psi_A(\vec{r}) \pm \psi_B(\vec{r})|^2$$

= $C_{\pm}^2 \int d^3r \left(|\psi_A(\vec{r})|^2 + |\psi_B(\vec{r})|^2 \pm 2\psi_A(\vec{r})\psi_B(\vec{r}) \right)$
= $C_{\pm}^2 (2 + 2S(R))$

where

$$R = \left| \vec{R}_A - \vec{R}_B \right| \tag{13.215}$$

$$S(R) = \int d^3 r \psi_A(\vec{r}) \psi_B(\vec{r}) = \left(1 + \frac{R}{a} + \frac{R^2}{3a^2}\right) e^{-\frac{R}{a}}$$
(13.216)

The expectation value of \hat{H} in these trial states is

$$\left\langle \hat{H} \right\rangle_{\pm} = \frac{1}{2 \pm 2S} \left(\left\langle A \right| \hat{H} \left| A \right\rangle + \left\langle B \right| \hat{H} \left| B \right\rangle \pm 2 \left\langle A \right| \hat{H} \left| B \right\rangle \right)$$
(13.217)

where

$$\langle A|\hat{H}|A\rangle = \int d^3r\psi_A(\vec{r})\hat{H}\psi_A(\vec{r}) \qquad (13.218)$$

and so on.

Now

$$\begin{split} \langle A|\hat{H}|A\rangle &= \int d^{3}r\psi_{A}(\vec{r}) \left(-\frac{\hbar^{2}}{2m} \nabla^{2} - \frac{e^{2}}{|\vec{r} - \vec{R}_{A}|} - \frac{e^{2}}{|\vec{r} - \vec{R}_{B}|} + \frac{e^{2}}{|\vec{R}_{A} - \vec{R}_{B}|} \right) \psi_{A}(\vec{r}) \\ &= \int d^{3}r\psi_{A}(\vec{r}) \left(-\frac{\hbar^{2}}{2m} \nabla^{2} - \frac{e^{2}}{|\vec{r} - \vec{R}_{A}|} \right) \psi_{A}(\vec{r}) \\ &+ \int d^{3}r\psi_{A}(\vec{r}) \left(\frac{e^{2}}{|\vec{R}_{A} - \vec{R}_{B}|} \right) \psi_{A}(\vec{r}) - \int d^{3}r\psi_{A}(\vec{r}) \left(\frac{e^{2}}{|\vec{r} - \vec{R}_{B}|} \right) \psi_{A}(\vec{r}) \\ &= E_{1} + \frac{e^{2}}{R} - \frac{e^{2}}{R} \left[1 - \left[1 + \frac{R}{a} \right] e^{-\frac{2R}{a}} \right] = E_{1} + \frac{e^{2}}{R} \left[1 + \frac{R}{a} \right] e^{-\frac{2R}{a}} \\ &= \langle B|\hat{H}|B \rangle \end{split}$$

where

 $E_1 =$ ground state energy of a hydrogen atom = -1 Ry (13.219)

In a similar way

$$\langle A | \hat{H} | B \rangle = \int d^3 r \psi_A(\vec{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{|\vec{r} - \vec{R}_A|} - \frac{e^2}{|\vec{r} - \vec{R}_B|} + \frac{e^2}{|\vec{R}_A - \vec{R}_B|} \right) \psi_B(\vec{r})$$

= $\left(E_1 + \frac{e^2}{R} \right) S(R) - \frac{e^2}{a} \left[1 + \frac{R}{a} \right] e^{-\frac{R}{a}}$

Putting everything together we get

$$\varepsilon_{\pm}(R) = \left\langle \hat{H} \right\rangle_{\pm}$$
(13.220)
= $\frac{1}{1 \pm S} \left[E_1 + \frac{e^2}{R} \left[1 + \frac{R}{a} \right] e^{-\frac{2R}{a}} \pm \left(E_1 + \frac{e^2}{R} \right) S(R) \mp \frac{e^2}{a} \left[1 + \frac{R}{a} \right] e^{-\frac{R}{a}} \right]$

A plot of $\varepsilon_{\pm}(R)$ versus R/a is shown in Figure 13.9 below.

The top curve represents $\varepsilon_{-}(R)$ and the bottom curve is $\varepsilon_{+}(R)$. It is clear that $\varepsilon_{+}(R)$ has a minimum and $\varepsilon_{-}(R)$ does not.

Therefore, the symmetric wave function leads to *binding* between the nuclei and the antisymmetric wave function does not.

In the region between the nuclei

$$\psi_{+}(\vec{r}) >> \psi_{-}(\vec{r})$$
 (13.221)

In fact, $\psi_{-}(\vec{r})$ is zero on the bisecting plane. This implies that $\psi_{+}(\vec{r})$ gives the larger probability for the electron to be between the nuclei. *This is the binding mechanism.* In this state the electron has the greatest attraction from *both*



Figure 13.9: $\varepsilon_{\pm}(R)$ versus R/a

protons.

This theory implies

$$\psi_+(\vec{r})$$
 minimum \rightarrow nuclear separation = 1.3
minimum energy = -1.76 eV

The experimental results are

nuclear separation = 1.06minimum energy $= -2.8 \ eV$

A single electron wave function $\psi_{\pm} = C_{\pm} [\psi_A(\vec{r}) \pm \psi_B(\vec{r})]$ is a molecular orbital. Our assumption of a linear combination or these atomic orbitals comprises the LCAO model.

> $\psi_+(\vec{r})$ state \rightarrow binding \rightarrow binding orbital $\psi_-(\vec{r})$ state $\rightarrow E > 0$ always \rightarrow antibinding orbital

Hydrogen Molecule (H_2)

We now have two electrons. The Hamiltonian for the two electrons in the H_2 molecule is

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 - \frac{e^2}{\left|\vec{r}_1 - \vec{R}_A\right|} - \frac{e^2}{\left|\vec{r}_1 - \vec{R}_B\right|} - \frac{e^2}{\left|\vec{r}_2 - \vec{R}_A\right|} - \frac{e^2}{\left|\vec{r}_2 - \vec{R}_B\right|} + \frac{e^2}{\left|\vec{r}_1 - \vec{r}_2\right|} + \frac{e^2}{\left|\vec{R}_A - \vec{R}_B\right|}$$
(13.222)

There are two different variational approaches to the solution of this problem.

Molecular Orbital Method

We make the assumption that the wave function of the two electrons in the ground state is

$$\psi_{symm}(1,2) = \psi_{+}(1)\psi_{+}(2)\chi_{spin-singlet}$$

$$= \frac{1}{2(1+S(R))} \left(\psi_{A}(1) + \psi_{B}(1)\right) \left(\psi_{A}(2) + \psi_{B}(2)\right) \chi_{singlet}$$
(13.223)

This wave function has a symmetric spatial part and an antisymmetric spin part so that the total wave function for the two electrons is antisymmetric. The spatial part is the product of the H_2^+ molecular wave functions. The spatial part has been chosen to be a binding orbital since it is maximum in between the nuclei. Therefore, we expect this spatial wave function to represent the ground state of the H_2 molecule. The choice of the singlet spin function (paired spins) is solely to insure antisymmetry.

The triplet spin state is symmetric an requires an antisymmetric spatial part, i.e.,

$$\psi_{anti}(1,2) = \frac{1}{\sqrt{2}} \left[\psi_+(1)\psi_-(2) - \psi_-(1)\psi_+(2) \right] \chi_{triplet}$$
(13.224)

This spatial part is an antibinding orbital since it is zero in between the nuclei and thus has a higher energy than the other wave function. These assumptions clearly have defects:

- 1. At small proton separations the wave function is the product of two 1s hydrogen wave functions instead of approximating a helium wavefunction, i.e., the system is like helium with Z = 2 at small separations, but our approximation assumes two electrons in S-states with Z = 1.
- 2. At larger proton separations there is little probability that the two electrons will both be near the same proton. If we expand out the spatial part of the wave function we have

 $(\psi_A(1)\psi_A(2) + \psi_B(1)\psi_B(2)) + (\psi_A(1)\psi_B(2) + \psi_A(2)\psi_B(1))$

the first term says the two electrons are near the same proton. The last term implies that one electron is near each proton. The presence of the first term with the same amplitude as the second term is a poor approximation.

This last argument simply reflects the fact that at large proton separations

H + H is more energetically favorable then $p + H^{-}$

The assumed wave function will still give a reasonable upper bound for the binding energy since it depends only on the behavior of the system near the actual nuclear separations, which is in between the above two extremes.

The Heitler-London or Valence Bond Method

In this method we leave out the $\psi_A(1)\psi_A(2)$ and $\psi_B(1)\psi_B(2)$ terms. We choose

$$\psi_s(1,2) = \frac{1}{\sqrt{2(1+S^2)}} \left(\psi_A(1)\psi_B(2) + \psi_A(2)\psi_B(1)\right)\chi_{\sin g}$$
(13.225)

$$\psi_t(1,2) = \frac{1}{\sqrt{2(1-S^2)}} \left(\psi_A(1)\psi_B(2) - \psi_A(2)\psi_B(1)\right)\chi_{trip}$$
(13.226)

In this case, for large separations we have separated hydrogen atoms, which is the correct physics. These wave functions exhibit the same small separation problems as in the molecular orbital method, however.

The expectation value of \hat{H} in these states is

$$\varepsilon_{\pm}(R) = \langle \hat{H} \rangle_{\pm}$$

$$= \frac{\langle AB | \hat{H} | AB \rangle + \langle BA | \hat{H} | BA \rangle \pm \langle AB | \hat{H} | BA \rangle \pm \langle BA | \hat{H} | AB \rangle}{2 \pm 2S^{2}}$$

$$= \frac{\langle AB | \hat{H} | AB \rangle \pm \langle AB | \hat{H} | BA \rangle}{1 \pm S^{2}}$$
(13.227)

where we have used

$$\langle AB | \hat{H} | AB \rangle = \langle BA | \hat{H} | BA \rangle$$

$$\langle AB | \hat{H} | BA \rangle = \langle BA | \hat{H} | AB \rangle$$

The + sign is the singlet value and the - sign is the triplet value. The matrix elements are given by

$$\langle AB|\hat{H}|AB\rangle = \int d^3r_1 d^3r_2 \psi_A(1)\psi_B(2)\hat{H}\psi_A(1)\psi_B(2)$$
(13.228)

$$\langle AB|\hat{H}|BA\rangle = \int d^3r_1 d^3r_2 \psi_A(1)\psi_B(2)\hat{H}\psi_A(2)\psi_B(1)$$
(13.229)

The Schrodinger equation for each of the 1S wave functions (ψ_A and ψ_B) is of the form

$$\left(-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{e^2}{\left|\vec{r}_1 - \vec{R}_A\right|}\right)\psi_A(\vec{r}_1) = E_1\psi_A(\vec{r}_1)$$
(13.230)

We therefore get for the matrix elements

$$\langle AB|\hat{H}|AB\rangle = 2E_1 + Q \tag{13.231}$$

$$\langle AB | \hat{H} | BA \rangle = S^2 (2E_1 + \frac{e^2}{R}) + \tilde{Q}$$
 (13.232)

where

Q = total Coulomb energy

$$= \int d^{3}r_{1}d^{3}r_{2}\psi_{A}^{2}(1)\psi_{B}^{2}(2)\left[\frac{e^{2}}{|\vec{r}_{1}-\vec{r}_{2}|} - \frac{e^{2}}{|\vec{r}_{1}-\vec{R}_{B}|} - \frac{e^{2}}{|\vec{r}_{2}-\vec{R}_{A}|} + \frac{e^{2}}{|\vec{R}_{A}-\vec{R}_{B}|}\right]$$
$$= -2\int d^{3}r_{1}\psi_{A}^{2}(1)\left[\frac{e^{2}}{|\vec{r}_{1}-\vec{R}_{B}|}\right] + \int d^{3}r_{1}d^{3}r_{2}\psi_{A}^{2}(1)\psi_{B}^{2}(2)\left[\frac{e^{2}}{|\vec{r}_{1}-\vec{r}_{2}|}\right] + \frac{e^{2}}{R}$$
$$= V_{C}(\vec{R}) + \frac{e^{2}}{R}$$
(13.233)

 \tilde{Q} = total exchange energy

$$= \int d^{3}r_{1}d^{3}r_{2}\psi_{A}(1)\psi_{B}(2)\psi_{A}(2)\psi_{B}(1)\left[\frac{e^{2}}{|\vec{r}_{1}-\vec{r}_{2}|}-\frac{e^{2}}{|\vec{r}_{1}-\vec{R}_{B}|}-\frac{e^{2}}{|\vec{r}_{2}-\vec{R}_{A}|}\right]$$

$$= -2\int d^{3}r_{1}\psi_{A}(1)\psi_{B}(1)\left[\frac{e^{2}}{|\vec{r}_{1}-\vec{R}_{A}|}\right]$$

$$+\int d^{3}r_{1}d^{3}r_{2}\psi_{A}(1)\psi_{B}(2)\psi_{A}(2)\psi_{B}(1)\left[\frac{e^{2}}{|\vec{r}_{1}-\vec{r}_{2}|}\right]+S^{2}\frac{e^{2}}{R}$$

$$= V_{ex}(\vec{R})+S^{2}\frac{e^{2}}{R}$$
(13.234)

The exchange term is a measure of the overlap of the wave functions, weighted by the potential energies. It is the result of an interplay between quantum mechanics and the PEP. Putting everything together we have

$$\varepsilon_{\pm} = 2E_1 + \frac{V_C \pm V_{ex}}{1 \pm S^2} + \frac{e^2}{R} = 2E_1 + \frac{\left(V_C + \frac{e^2}{R}\right) \pm \left(V_{ex} + S^2 \frac{e^2}{R}\right)}{1 \pm S^2}$$
(13.235)

We have

$$V_C + \frac{e^2}{R} > 0$$
 always and $V_{ex} + S^2 \frac{e^2}{R} < 0$ generally (13.236)

which implies that $\varepsilon_+ < \varepsilon_-$. In fact, one finds that

- $\varepsilon_{-}-2E_{1}$ has no minimum
- $\varepsilon_+ 2 E_1$ has a minimum 30 eV deep at $R = 1.5 a_0$

as shown in Figure 13.10 below.



Figure 13.10: Energy versus R

This implies that the molecule binds in the singlet state but not in the triplet state. One finds that the strength of the binding is proportional to the overlap of the two electron states .

The triplet wave function spatial part vanishes if both electrons are in between the protons implying a smaller overlap and thus no binding.

13.2.4 Vibrational and Rotational Levels of a Molecule

We found earlier that the nuclear wave functions satisfy an equation of the form

$$(\hat{T}_N + \varepsilon_n(\vec{R}))\psi_n(\vec{R}) = E\psi_n(\vec{R})$$
(13.237)

if we consider a two-atom molecule like HCL, this equation gives the rotational and vibrational energy levels.

If we denote the relative coordinate of the nuclei by \vec{r} , we have

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \varepsilon(r)\right)\psi(\vec{r}) = E\psi(\vec{r})$$
(13.238)

where

$$r = |\vec{r}|$$
 and $m = \frac{M_1 M_2}{M_1 + M_2}$ = reduced mass (13.239)

We have used the fact that the effective potential depends only on r.

This represents a rotationally symmetric problem (central force field). Therefore, we assume

$$\psi(\vec{r}) = R_{n\ell}(r)Y_{\ell m}(\theta,\varphi) \tag{13.240}$$

Substitution gives

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \varepsilon(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)R_{n\ell}(r) = ER_{n\ell}(r)$$
(13.241)

Defining

$$V_{eff}(r) = \varepsilon(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$
(13.242)

and using

$$u_{n\ell}(r) = rR_{n\ell}(r)$$
 (13.243)

we have

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{eff}(r)\right)u_{n\ell}(r) = Eu_{n\ell}(r)$$
(13.244)

For small values of ℓ , $V_{eff}(r)$ has a minimum that depends on ℓ (say at $r = r_{\ell}$). In the neighborhood of this minimum, we can expand $V_{eff}(r)$ in a Taylor series

$$V_{eff}(r) = V_{eff}(r_{\ell}) + \frac{1}{2}m\omega_{\ell}^{2}(r - r_{\ell})^{2} + \dots$$
(13.245)

where

$$m\omega_{\ell}^2 = \left(\frac{d^2 V_{eff}}{dr^2}\right)_{r=r_{\ell}}$$
(13.246)

For small displacements from equilibrium, we have simple harmonic motion. Letting $q=r-r_\ell$ we get

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \varepsilon(r_\ell) + \frac{\hbar^2\ell(\ell+1)}{2mr_\ell^2} + \frac{1}{2}m\omega_\ell^2 q^2\right)u_{n\ell}(r) = Eu_{n\ell}(r)$$
(13.247)

where we have put $r = r_{\ell}$ (small displacement) in

$$\varepsilon(r) \text{ and } \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$
 (13.248)

We end up with the harmonic oscillator equation where the energy is

$$E = \varepsilon(r_{\ell}) + \frac{\hbar^2 \ell(\ell+1)}{2I_{\ell}} + \hbar \omega_{\ell}(n+1/2)$$
 (13.249)

with

$$I_{\ell} = mr_{\ell}^2 = \text{ effective moment of inertia}$$
 (13.250)

The corresponding stationary states are

$$u_{n\ell} = A_n H_n \left(\frac{q}{q_{0\ell}}\right) \exp\left\{-\frac{1}{2} \left(\frac{q}{q_{0\ell}}\right)^2\right\}$$
(13.251)

where

$$q_{0\ell} = \left(\frac{\hbar}{m\omega_\ell}\right)^{1/2} \tag{13.252}$$

Although the wave functions do not satisfy the requirement u(r = 0) = 0, the energy eigenvalues are still reasonably accurate in this approximations, i.e.,

$$u_{n\ell}(0) \approx H_n(0) \exp\left\{-\frac{1}{2} \left(\frac{r_\ell}{q_{0\ell}}\right)^2\right\}$$
(13.253)

With $r_{\ell} \gg q_{0\ell}$, u(0) is very small. The energy eigenvalues contain contributions from

- 1. the effective electronic energy
- 2. the rotational energy
- 3. the vibrational energy

The rotational levels have $\lambda \approx 0.1 - 1 \ cm$ which corresponds to the far infrared and microwave regions. The vibrational levels have $\lambda \approx 2 \times 10^{-3} - 3 \times 10^{-3} \ cm$ which corresponds to the infrared region.

13.3 Problems

13.3.1 S-Wave Phase Shift

We wish to find an approximate expression for the s-wave phase shift, δ_0 , for scattering of low energy particles from the potential

$$V(r) = \frac{C}{r^4} \quad , \quad C > 0$$

(a) For low energies, $k \approx 0$, the radial Schrodinger equation for $\ell = 0$ may be approximated by (dropping the energy term):

$$\left[-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{2mC}{\hbar^2r^4}\right]R^{inside}_{\ell=0}(r) = 0$$

By making the transformations

$$R(r) = \frac{1}{\sqrt{r}}\varphi(r)$$
, $r = \frac{i}{\hbar}\frac{\sqrt{2mC}}{x}$

show that the radial equation may be solved in terms of Bessel functions. Find an approximate solution, taking into account behavior at r = 0. (b) Using the standard procedure of matching this to $R_{\ell=0}^{outside}(r)$ at r = a (where a is chosen such that $\hbar a \gg \sqrt{2mC}$ and $ka \ll 1$) show that

$$\delta_0 = -k \frac{\sqrt{2mC}}{\hbar}$$

which is independent of a.

13.3.2 Scattering Slow Particles

Determine the total cross section for the scattering of slow particles (ka < 1) by a potential $V(r) = C\delta(r-a)$.

13.3.3 Inverse square scattering

Particles are scattered from the potential

$$V(r) = \frac{g}{r^2}$$

where g is a positive constant.

- (a) Write the radial wave equation and determine the regular solutions.
- (b) Prove that the phase shifts are given by

$$\delta_{\ell} = \frac{\pi}{2} \left[\ell + \frac{1}{2} - \sqrt{\left(\ell + \frac{1}{2}\right)^2 + \frac{2\mu g}{\hbar^2}} \right]$$

- (c) Find the energy dependence of the differential cross section for a fixed scattering angle.
- (d) Find δ_{ℓ} for $2\mu g/\hbar^2 \ll 1$ and show that the differential cross section is

$$\frac{d\sigma}{d\theta} = \frac{\pi^3}{2\hbar^2} \frac{g^2 \mu}{E} \cot\left(\frac{\theta}{2}\right)$$

where E is the energy of the scattered particle.

(e) For the same potential, calculate the differential cross section using the Born approximation and compare it with the above results. Why did this happen?

13.3.4 Ramsauer-Townsend Effect

What must $V_0 a^2$ be for a 3-dimensional square well potential in order that the scattering cross section be zero in the limit of zero bombarding energy (Ramsauer-Townsend effect)?

13.3.5 Scattering from a dipole

Consider an electric dipole consisting of two electric charges e and -e at a mutual distance 2a. Consider also a particle of charge e and mass m with an incident wave vector \vec{k} perpendicular to the direction of the dipole, i.e., choose the incident particle along the z-axis $\vec{k} = k\hat{z}$ and the dipole set along he x-axis or the charges are at $\pm a\hat{x}$.

Calculate the scattering amplitude in Born approximation, Find the directions at which the differential cross-section is maximum.

13.3.6 Born Approximation Again

- (a) Evaluate, in the Born approximation, the differential cross section for the scattering of a particle of mass m by a delta-function potential $V(\vec{r}) = B\delta(\vec{r})$.
- (b) Comment on the angular and velocity dependence.
- (c) Find the total cross section.

13.3.7 Translation invariant potential scattering

Show that if the scattering potential has a translation invariance property $V(\vec{r} + \vec{R}) = V(\vec{r})$, where \vec{R} is a constant vector, then the Born approximation scattering vanishes unless $\vec{q} \cdot \vec{R} = 2\pi n$, where n is an integer and \vec{q} is the momentum transfer. This corresponds to scattering from a lattice. For any vector \vec{R} of the lattice, the set of vectors \vec{k} that satisfy $\vec{k} \cdot \vec{R} = 2\pi n$ constitutes the *reciprocal lattice*. This prove then shows that the scattering amplitude vanishes unless the momentum transfer \vec{q} is equal to some vector of the reciprocal lattice. This is the *Bragg-Von Laue* scattering condition.

13.3.8 $\ell = 1$ hard sphere scattering

Consider the hard sphere potential of the form

$$V(r) = \begin{cases} 0 & r > r_0 \\ \infty & r < r_0 \end{cases}$$

where $kr_0 \ll 1$. Write the radial Schrödinger equation for $\ell = 1$, and show that the solution for the p-wave scattering is of the form

$$\chi_{k1}(r) = rR_{k1}(r) = A\left[\frac{\sin(kr)}{kr} - \cos(kr) + a\left(\frac{\cos(kr)}{kr} + \sin(kr)\right)\right]$$

where A and a are constants. Determine $\delta_1(k)$ from the condition imposed on $\chi_{k1}(r_0)$. Show that in the limit $k \to 0$, $\delta_1(k) \approx (kr_0)^3$ and $\delta_1(k) \ll \delta_0(k)$.

13.3.9 Vibrational Energies in a Diatomic Molecule

The nuclei of a diatomic molecule are moving in a potential field given as

$$V_{eff}(R) = -2D\left[\left(\frac{a_0}{R}\right) - \left(\frac{a_0}{R}\right)^2\right] + \left(\frac{\hbar^2}{2\mu R^2}\right)J(J+1)$$

Express this potential near its minimum by a harmonic oscillator potential and determine the vibrational energies of the molecule.

13.3.10 Ammonia Molecule

In the ammonia molecule, NH_3 , the three hydrogen atoms lie in a plane at the vertices of an equilateral triangle. The single nitrogen atom can lie either above or below the plane containing the hydrogen atoms, but in either case the nitrogen atom is equidistant from each of the hydrogen atoms (they form an equilateral tetrahedron). Let us call the state of the ammonia molecule when the nitrogen atom is above the plane of the hydrogen atoms $|1\rangle$ and let us call the state of the ammonia molecule when the nitrogen atom is below the plane of the hydrogen atoms $|2\rangle$.

How do we determine the energy operator for the ammonia molecule? If these were the energy eigenstates, they would clearly have the same energy (since we cannot distinguish them in any way). So diagonal elements of the energy operator must be equal if we are using the $(|1\rangle, |2\rangle)$ basis. But there is a small probability that a nitrogen atom above the plane will be found below the plane and vice versa (called tunneling). So the off-diagonal element of the energy operator must not be zero, which also reflects the fact that the *above* and *below* states are not energy eigenstates. We therefore arrive with the following matrix as representing the most general possible energy operator for the ammonia molecule system:

$$\hat{H} = \left(\begin{array}{cc} E_0 & A \\ A & E_0 \end{array}\right)$$

where E_0 and A are constants.

- (a) Find the eigenvalues and eigenvectors of the energy operator. Label them as $(|I\rangle, |II\rangle)$
- (b) Let the initial state of the ammonia molecule be |I⟩, that is, |ψ(0)⟩ = |I⟩. What is |ψ(t)⟩, the state of the ammonia molecule after some time t? What is the probability of finding the ammonia molecule in each of its energy eigenstates? What is the probability of finding the nitrogen atom above or below the plane of the hydrogen atoms?
- (c) Let the initial state of the ammonia molecule be $|1\rangle$, that is, $|\psi(0)\rangle = |1\rangle$. What is $|\psi(t)\rangle$, the state of the ammonia molecule after some time t? What is the probability of finding the ammonia molecule in each of its energy eigenstates? What is the probability of finding the nitrogen atom above or below the plane of the hydrogen atoms?

13.3.11 Ammonia molecule Redux

Treat the ammonia molecule shown in the figure



Figure 13.11: Ammonia Molecule

as a symmetric rigid rotator. Call the moment of inertia about the z-axis I_3 and the moments about the pairs of axes perpendicular to the z-axis I_1 .

- (a) Write down the Hamiltonian of this system in terms of \vec{L} , I_3 and I_1 .
- (b) Show that $\left[\hat{H}, \hat{L}_z\right] = 0$
- (c) What are the eigenstates and eigenvalues of the Hamiltonian?
- (d) Suppose that at time t = 0 the molecule is in the state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|0,0\rangle + \frac{1}{\sqrt{2}}|1,1\rangle$$

What is $|\psi(t)\rangle$?

13.3.12 Molecular Hamiltonian

A molecule consists of three atoms located on the corners of an equilateral triangle as shown below



Figure 13.12: A Molecule

The eigenstates of the molecule can be written as linear combinations of the atomic states $|\alpha_i\rangle$, i = 1, 2, 3, such that

$$\langle \alpha_i | \hat{H} | \alpha_j \rangle = \begin{cases} \varepsilon & \text{if } i = j \\ -\beta & \text{if } i \neq j \end{cases}$$

where \hat{H} is the Hamiltonian and $\varepsilon, \beta > 0$. Now define an operator \hat{R} such that

$$\hat{R} |\alpha_1\rangle = |\alpha_2\rangle$$
 , $\hat{R} |\alpha_2\rangle = |\alpha_3\rangle$, $\hat{R} |\alpha_3\rangle = |\alpha_1\rangle$

- (a) Show that \hat{R} commutes with \hat{H} and find the eigenvalues and eigenvectors of \hat{R} .
- (b) Find the eigenvalues and eigenvectors of \hat{H} .

13.3.13 Potential Scattering from a 3D Potential Well

A 3D stepwise constant potential is given by

$$V(\vec{r}) = \begin{cases} V_1 & 0 < |\vec{r}| < R_1 \\ V_2 & R_1 < |\vec{r}| < R_2 \end{cases}$$

and zero outside R_2 .

- (1) Calculate the differential cross-section in the Born approximation as a function of the momentum transfer q, where $\vec{q} = \vec{k}' \vec{k}$.
- (2) Verify your expression is correct by showing that it reduces to the result for the *spherical square well* when $V_1 = V_2$, i.e., calculate separately the spherical square well result and set $V_1 = V_2 \rightarrow V_0$.
- (3) Plot the result of the square well(part(2)) as a function of qR_2 over a sufficient region to understand its behavior (i.e., $qR_2 \rightarrow 0$, $qR_2 \sim 1$, $qR_2 \gg 1$). Note and explain any noteworthy features.
- (4) Now plot not simply versus q, but versus θ , $0 < \theta < \pi$, for four representative values of the energy. Use atomic scales: $R_2 = 3a_B$, $V_0 = 1 Ry$. You have to decide on relevant energies to plot; it should be helpful to plot on the same graph with different line styles or colors.
- (5) Return to the potential of part(1). Let $R_2 = 2^{1/3}R_1$, so there is an equal volume inside R_1 and between R_1 and R_2 . Then set $V_1 = -V_2$, this means the volume integral of the potential vanishes, and also that it has strong \vec{r} dependence (step function). Determine the differential cross-section in this case. Plot versus energy and angle.
- (6) Finally, consider a Gaussian potential that has the same range parameter and the same volume integral as the simple square well of part(2). Calculate the differential cross-section in this case. Can you identify possible effects due to the sharp structure (discontinuity) that occurs in only one of them.

13.3.14 Scattering Electrons on Hydrogen

From measurements of the differential cross section for scattering electrons off protons (in atomic hydrogen) it was found that the proton had a charge density given by

$$\rho(r) = ae^{-br}$$

where a and b are constants.

- (a) Find a and b such that the proton charge equals e, the charge on the electron.
- (b) Show that the proton mean square radius is given by

$$\left\langle r^2 \right\rangle = \frac{12}{b^2}$$

(c) Assuming a reasonable value for $\langle r^2 \rangle^{1/2}$ calculate *a* in esu/cm^2 .

13.3.15 Green's Function

Consider a particle of mass m which scatters off a potential V(x) in one dimension.

(a) Show that the free-particle Green's function for the time-independent Schrodinger equation with energy E and outgoing-wave boundary conditions is

$$G_E(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \frac{e^{ikx}}{E - \frac{\hbar^2 k^2}{2m} + i\varepsilon}$$

with ε a positive infinitesimal.

(b) Write that the equation for the energy eigenfunction corresponding to an incident wave traveling in the positive x-direction. Using this equation find the reflection probability in the first Born approximation for the potential

$$V(x) = \begin{cases} V_0 & |x| < a/2 \\ 0 & |x| > a/2 \end{cases}$$

For what values of E do you expect this to be a good approximation?

13.3.16 Scattering from a Hard Sphere

In this case we have

$$V(x) = \begin{cases} 0 & r > b \\ \infty & r \le b \end{cases}$$

which is a repulsive potential. Determine the low energy differential and total cross sections. Discuss your results.

13.3.17 Scattering from a Potential Well

In this case

$$V(x) = \begin{cases} 0 & r > b \\ V_0 & r \le b \end{cases}$$

Determine δ_0 , the total cross section and the existence of resonances.

13.3.18 Scattering from a Yukawa Potential

Use the Born approximation to determine the differential cross section for a Yukawa potential

$$V(\vec{r}) = a \frac{e^{-\mu r}}{r}$$

Discuss the limit $\mu \to 0$.

13.3.19 Born approximation - Spin-Dependent Potential

Use the Born approximation to determine the differential cross section for the spin-dependent potential

$$V(\vec{r}) = e^{-\mu r^2} \left[A + B\vec{\sigma} \cdot \vec{r} \right]$$

13.3.20 Born approximation - Atomic Potential

Use the Born approximation to determine the differential cross section for the atomic potential seen by an incoming electron, which can be represented by the function

$$V(r) = -Ze^2 \int \frac{\rho_T(\vec{r}')d^3\vec{r}'}{|\vec{r} - \vec{r}'|}$$

where

$$\rho_T(\vec{r}') = \rho_{nuclear}(\vec{r}') + \rho_{electronic}(\vec{r}') = \delta(\vec{r}') - \rho(\vec{r}')$$

13.3.21 Lennard-Jones Potential

Consider the *Lennard-Jones* potential (shown below) used to model the binding of two atoms into a molecule.



Figure 13.13: Lennard-Jones Potential

It is given by

$$V(r) = \frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}$$

(a) Near the minimum r_0 , the potential looks harmonic. Including the first anharmonic correction, show that up to a constant term

$$V(x) = \frac{1}{2}m\omega^2 x^2 + \xi x^3$$

where $r_0 = (2C_{12}/C_6)^{1/6}$, $x = r - r_0$, $m\omega^2/2 = V''(r_0)$ and $\xi = V'''(r_0)/6$.
Let us write $\hat{H} = \hat{H}_0 + \hat{H}_1$, where $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2$ and $\hat{H}_1 = \xi x^3$.

(b) What is the small parameter of the perturbation expansion?

- (c) Show that the first energy shift vanishes (use symmetry).
- (d) Show that the second energy shift (first nonvanishing correction) is

$$E_n^{(2)} = \frac{\xi^2 \left(\frac{\hbar}{2m\omega}\right)^3}{\hbar\omega} \sum_{m \neq n} \frac{\left|\langle m | \left(\hat{a} + \hat{a}^+\right)^3 | n \rangle\right|^2}{n - m}$$

(e) Evaluate the matrix elements to show that

$$E_n^{(2)} = \frac{\xi^2 \hbar^2}{m^3 \omega^4} \left[\frac{(n-2)(n-1)(n)}{3} + \frac{(n+3)(n+2)(n+1)}{-3} + \frac{9n^3}{1} + \frac{9(n+1)^3}{-1} \right]$$
$$= -\frac{\xi^2 \hbar^2}{m^3 \omega^4} \left[\frac{15}{4} (n+1/2)^2 + \frac{7}{16} \right]$$

(f) Consider carbon C-C bonds take Lennard-Jones parameters $C_6 = 15.2 \ eV^{6}$ and $C_{12} = 2.4 \times 10^4 \ eV^{-12}$. Plot the potential and the energy levels from the ground to second excited state including the anharmonic shifts.


Figure 13.14: Diatomic Molecule

13.3.22 Covalent Bonds - Diatomic Hydrogen

Consider the simplest neutral molecule, diatomic hydrogen H_2 , consisting of two electrons and two protons.

- (a) Classically, where would you put the electrons so that the nuclei are *attracted* to one another in a bonding configuration? What configuration maximally repels the nuclei (anti-bonding)?
- (b) Consider the two-electron state of this molecule. When the nuclei are far enough apart, we can construct this state out of *atomic orbitals* and spins. Write the two possible states as products of orbital and spin states. Which is the *bonding* configuration? Which is the *anti-bonding*?
- (c) Sketch the potential energy seen by the nuclei as a function of the internuclear separation R for the two different electron configurations. Your *bonding configuration* should allow for bound-states of the nuclei to one another. This is the *covalent bond*.

13.3.23 Nucleus as sphere of charge - Scattering

To a first approximation, the potential that a charged particle feels from a hydrogen atom can be thought of as due to a positive point charge at the origin (the proton) plus a uniform region of negative charge occupying a sphere of radius a_0 (the so-called electron cloud).

- (a) Calculate, in the Born approximation, the differential cross section for scattering a charged particle from the hydrogen atom as modeled above (neglect the recoil of the hydrogen atom).
- (b) What is the form of the differential cross section for low energy? Compare with the pure Coulomb cross section.
- (c) Show that the differential cross section becomes more and more like a pure Coulomb cross section as the energy of the incident particle increases. Explain why this happens.

Chapter 14

Some Examples of Quantum Systems

14.1 Coherent and Squeezed States

We have derived relationships between the non-Hermitian operators \hat{a} and \hat{a}^{\dagger} and the position and momentum operators

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^+ + \hat{a}) \quad , \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}} (\hat{a}^+ - \hat{a}) \tag{14.1}$$

Working with the coherent states defined by

$$\hat{a} \left| \alpha \right\rangle = \alpha \left| \alpha \right\rangle \tag{14.2}$$

we found

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} |m\rangle$$
(14.3)

where

$$\left|\alpha^{2}\right| = N = \left<\alpha\right|\hat{N}_{op}\left|\alpha\right>$$
(14.4)

Let us now derive some important relations.

$$\langle \alpha | \hat{x} | \alpha \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle \alpha | (\hat{a}^{+} + \hat{a}) | \alpha \rangle$$
$$= \sqrt{\frac{\hbar}{2m\omega}} (\alpha + \alpha^{*}) = \sqrt{\frac{2\hbar}{m\omega}} \text{Real}(\alpha)$$
(14.5)

$$\langle \alpha | \hat{p} | \alpha \rangle = i \sqrt{\frac{\hbar m \omega}{2}} \langle \alpha | (\hat{a}^{+} - \hat{a}) | \alpha \rangle$$

= $i \sqrt{\frac{\hbar m \omega}{2}} (\alpha^{*} - \alpha) = \sqrt{2m\hbar\omega} \text{Imag}(\alpha)$ (14.6)

$$\langle \alpha | \hat{x}^{2} | \alpha \rangle = \frac{\hbar}{2m\omega} \langle \alpha | (\hat{a}^{+} \hat{a}^{+} + \hat{a} \hat{a}^{+} + \hat{a}^{+} \hat{a} + \hat{a} \hat{a}) | \alpha \rangle$$

$$= \frac{\hbar}{2m\omega} \langle \alpha | (\alpha^{*2} + \alpha \alpha^{*} + \alpha^{*} \alpha + \alpha^{2} + 1) | \alpha \rangle$$

$$= \langle \alpha | \hat{x} | \alpha \rangle^{2} + \frac{\hbar}{2m\omega}$$

$$(14.7)$$

$$\langle \alpha | \hat{p}^{2} | \alpha \rangle = -\frac{\hbar m \omega}{2} \langle \alpha | (\hat{a}^{*} \hat{a}^{*} - \hat{a} \hat{a}^{*} - \hat{a}^{*} \hat{a} + \hat{a} \hat{a}) | \alpha \rangle$$

$$= -\frac{\hbar m \omega}{2} \langle \alpha | (\alpha^{*2} - \alpha \alpha^{*} - \alpha^{*} \alpha + \alpha^{2} - 1) | \alpha \rangle$$

$$= \langle \alpha | \hat{p} | \alpha \rangle^{2} + \frac{\hbar m \omega}{2}$$

$$(14.8)$$

Using these relations we have

$$(\Delta x)^{2} = \langle \alpha | \hat{x}^{2} | \alpha \rangle - \langle \alpha | \hat{x} | \alpha \rangle^{2} = \frac{\hbar}{2m\omega}$$
(14.9)

$$\left(\Delta p\right)^{2} = \left\langle \alpha \right| \hat{p}^{2} \left| \alpha \right\rangle - \left\langle \alpha \right| \hat{p} \left| \alpha \right\rangle = \frac{\hbar m \omega}{2} \tag{14.10}$$

Hence

$$\Delta x \Delta p = \frac{\hbar}{2} \tag{14.11}$$

which says that coherent states are minimum uncertainty states.

Now let us find the differential equation satisfied by $\langle x\,|\,\alpha\rangle$ and determine its solution. We have

$$\langle x | \hat{a} | \alpha \rangle = \alpha \langle x | \alpha \rangle = \frac{1}{2} \langle x | \left(\sqrt{\frac{2m\omega}{\hbar}} \hat{x} - \frac{\hat{p}}{i} \sqrt{\frac{2}{m\omega\hbar}} \right) | \alpha \rangle$$
$$= \frac{1}{2} \left(\sqrt{\frac{2m\omega}{\hbar}} \hat{x} - \frac{1}{i} \sqrt{\frac{2}{m\omega\hbar}} \left(-i\hbar \frac{d}{dx} \right) \right) \langle x | \alpha \rangle$$

 or

$$\left(\hat{x} + \frac{\hbar}{m\omega}\frac{d}{dx}\right)\langle x \mid \alpha \rangle = \sqrt{\frac{2\hbar}{m\omega}}\langle x \mid \alpha \rangle \tag{14.12}$$

which has the solution (check by substitution)

$$\langle x \mid \alpha \rangle = C \exp\left[-\frac{(x - \langle x \rangle)^2}{4(\Delta x)^2} + \frac{i}{\hbar} \langle p \rangle x\right]$$
 (14.13)

$$= C' \exp\left[-\frac{m\omega}{2\hbar} \left(x - \sqrt{\frac{2\hbar}{m\omega}}\alpha\right)^2\right]$$
(14.14)

For a fixed oscillator mode, specified by a given value of $m\omega$, the coherent states are the manifold of those minimum uncertainty states that have definite values of Δx and Δp . If $m\omega = 1$, then the uncertainties in x and p are both equal to $\sqrt{\hbar/2}$.

We can construct other minimum uncertainty states with a narrower Δx , the so-called *squeezed states*, for the same oscillator by defining a new set of raising and lowering operators.

$$\hat{b} = \sqrt{\frac{m\omega'}{2\hbar}} \left(\hat{x} + i\frac{\hat{p}}{m\omega'} \right) \quad , \quad \hat{b}^+ = \sqrt{\frac{m\omega'}{2\hbar}} \left(\hat{x} - i\frac{\hat{p}}{m\omega'} \right) \tag{14.15}$$

where we introduce an arbitrarily chosen positive parameter ω' . Now we have

$$\begin{bmatrix} \hat{b}, \hat{b}^{+} \end{bmatrix} = \frac{m\omega'}{2\hbar} \left(-\frac{i}{m\omega'} \begin{bmatrix} \hat{x}, \hat{p} \end{bmatrix} + \frac{i}{m\omega'} \begin{bmatrix} \hat{p}, \hat{x} \end{bmatrix} \right)$$
$$= -\frac{i}{\hbar} \begin{bmatrix} \hat{x}, \hat{p} \end{bmatrix} = -\frac{i}{\hbar} i\hbar = 1$$
(14.16)

We also have

$$\begin{split} \hat{b} &= \sqrt{\frac{m\omega'}{2\hbar}} \left(\hat{x} + i\frac{\hat{p}}{m\omega'} \right) \\ &= \sqrt{\frac{m\omega'}{2\hbar}} \left(\sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^{+}) + \frac{i}{m\omega'} i\sqrt{\frac{\hbar m\omega}{2}} (\hat{a}^{+} - \hat{a}) \right) \\ &= \left(\sqrt{\frac{m\omega'}{2\hbar}} \sqrt{\frac{\hbar}{2m\omega}} + \sqrt{\frac{m\omega'}{2\hbar}} \frac{i}{m\omega'} i\sqrt{\frac{\hbar m\omega}{2}} \right) \hat{a}^{+} \\ &+ \left(\sqrt{\frac{m\omega'}{2\hbar}} \sqrt{\frac{\hbar}{2m\omega}} - \sqrt{\frac{m\omega'}{2\hbar}} \frac{i}{m\omega'} i\sqrt{\frac{\hbar m\omega}{2}} \right) \hat{a} \\ &= \frac{1}{2} \left(\sqrt{\frac{\omega'}{\omega}} - \sqrt{\frac{\omega}{\omega'}} \right) \hat{a}^{+} + \frac{1}{2} \left(\sqrt{\frac{\omega'}{\omega}} + \sqrt{\frac{\omega}{\omega'}} \right) \hat{a} \\ &= \lambda \hat{a} + \nu \hat{a}^{+} \end{split}$$
(14.17)

where

$$\lambda = \frac{1}{2} \left(\sqrt{\frac{\omega'}{\omega}} - \sqrt{\frac{\omega}{\omega'}} \right) \quad , \quad \nu = \frac{1}{2} \left(\sqrt{\frac{\omega'}{\omega}} + \sqrt{\frac{\omega}{\omega'}} \right) \tag{14.18}$$

and therefore

$$\hat{b}^{+} = \lambda \hat{a}^{+} + \nu \hat{a} \tag{14.19}$$

since λ and ν are real. Algebra also shows that

$$\lambda^{2} - \nu^{2} = \frac{1}{4} \left[\frac{\omega'}{\omega} + \frac{\omega}{\omega'} - \frac{\omega'}{\omega} - \frac{\omega}{\omega'} + 2 + 2 \right] = 1$$
(14.20)

We now invert the transformation. We have

$$\lambda \hat{b} - \nu \hat{b}^{+} = \lambda^{2} \hat{a} + \lambda \nu \hat{a}^{+} - \lambda \nu \hat{a}^{+} - \nu^{2} \hat{a} = (\lambda^{2} - \nu^{2}) \hat{a} = \hat{a}$$
(14.21)

which then implies that

$$\lambda \hat{b}^+ - \nu \hat{b} = \hat{a}^+ \tag{14.22}$$

We define the eigenstates of the lowering operator \hat{b} by

$$\hat{b}\left|\beta\right\rangle = \beta\left|\beta\right\rangle \tag{14.23}$$

These new states are also minimum uncertainty states for x and p. We want to calculate

$$(\Delta x)^{2} = \langle x^{2} \rangle - \langle x \rangle^{2} \quad , \quad (\Delta p)^{2} = \langle p^{2} \rangle - \langle p \rangle^{2} \tag{14.24}$$

Now we have

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a} + \hat{a}^{+} \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left(\left(\lambda - \nu \right) \hat{b} + \left(\lambda - \nu \right) \hat{b}^{+} \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left(\lambda - \nu \right) \left(\hat{b} + \hat{b}^{+} \right)$$
(14.25)

and

$$\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} \left(\hat{a}^{+} - \hat{a}\right)$$

$$= i\sqrt{\frac{\hbar m\omega}{2}} \left(\left(\lambda + \nu\right)\hat{b}^{+} - \left(\lambda + \nu\right)\hat{b}\right)$$

$$= i\sqrt{\frac{\hbar m\omega}{2}} \left(\lambda + \nu\right) \left(\hat{b}^{+} - \hat{b}\right)$$
(14.26)

These equations imply that earlier derivation we did is the same with different multiplicative factors so that

$$\left(\Delta x\right)^2 = \frac{\hbar}{2m\omega} \left(\lambda - \nu\right)^2 \tag{14.27}$$

$$\left(\Delta p\right)^2 = \frac{\hbar m\omega}{2} \left(\lambda + \nu\right)^2 \tag{14.28}$$

and therefore

$$(\Delta x)^{2} (\Delta p)^{2} = \frac{\hbar^{2}}{4} (\lambda - \nu)^{2} (\lambda + \nu)^{2} = \frac{\hbar^{2}}{4} (\lambda^{2} - \nu^{2})^{2} = \frac{\hbar^{2}}{4}$$

It turns out that the operators \hat{a} and \hat{b} are related by a unitary transformation, i.e.,

$$\hat{b} = \hat{U}\hat{a}\hat{U}^+ \tag{14.29}$$

where

$$\hat{U} = \exp\left[\frac{\xi}{2} \left(\hat{a}^2 - \hat{a}^{+2}\right)\right]$$
(14.30)

and

$$e^{\xi} = \lambda + \nu \tag{14.31}$$

Proof:

$$\hat{U}\hat{a}\hat{U}^{+} = \exp\left[\frac{\xi}{2}\left(\hat{a}^{2} - \hat{a}^{+2}\right)\right]\hat{a}\exp\left[-\frac{\xi}{2}\left(\hat{a}^{2} - \hat{a}^{+2}\right)\right] = e^{\hat{B}}\hat{a}e^{-\hat{B}}$$
(14.32)

Using the identity derived earlier we have

$$e^{\hat{B}}\hat{a}e^{-\hat{B}} = \hat{a} + \left[\hat{B}, \hat{a}\right] + \frac{1}{2}\left[\hat{B}, \left[\hat{B}, \hat{a}\right]\right] + \frac{1}{6}\left[\hat{B}, \left[\hat{B}, \left[\hat{B}, \hat{a}\right]\right]\right] + \dots$$
(14.33)

Now with

$$\hat{B} = \frac{\xi}{2} \left(\hat{a}^2 - \hat{a}^{+2} \right) \tag{14.34}$$

we have

$$\begin{split} \left[\hat{B}, \hat{a}\right] &= \frac{\xi}{2} \left(\left[\hat{a}^{2}, \hat{a}\right] - \left[\hat{a}^{+2}, \hat{a}\right] \right) = -\frac{\xi}{2} \left[\hat{a}^{+2}, \hat{a}\right] = \xi \hat{a}^{+} \\ \left[\hat{B}, \left[\hat{B}, \hat{a}\right]\right] &= \frac{\xi}{2} \xi \left[\hat{a}^{2}, \hat{a}^{+}\right] = \xi^{2} \hat{a} \\ \left[\hat{B}, \left[\hat{B}, \left[\hat{B}, \hat{a}\right]\right]\right] &= \xi^{3} \hat{a}^{+} \end{split}$$

and so on.

Therefore

$$\hat{U}\hat{a}\hat{U}^{+} = \hat{a} + \xi\hat{a}^{+} + \frac{\xi^{2}}{2}\hat{a} + \frac{\xi^{3}}{6}\hat{a}^{+} + \dots$$

$$= \hat{a}\left(1 + \frac{\xi^{2}}{2!} + \frac{\xi^{4}}{4!} + \dots\right) + \hat{a}^{+}\left(\xi + \frac{\xi^{3}}{3!} + \frac{\xi^{5}}{5!} + \dots\right)$$
(14.35)

If we define

$$\lambda = \left(1 + \frac{\xi^2}{2!} + \frac{\xi^4}{4!} + \dots\right) \quad , \quad \nu = \left(\xi + \frac{\xi^3}{3!} + \frac{\xi^5}{5!} + \dots\right) \tag{14.36}$$

so that

$$e^{\xi} = \lambda + \nu \tag{14.37}$$

we have

$$\hat{U}\hat{a}\hat{U}^{+} = \lambda\hat{a} + \nu\hat{a}^{+} = \hat{b}$$
(14.38)

Finally, we have

```
\begin{split} \hat{a} & |coherent\rangle = \alpha & |coherent\rangle \\ \hat{b} & |squeezed\rangle = \beta & |squeezed\rangle \\ \hat{U}\hat{a} & |coherent\rangle = \alpha \hat{U} & |coherent\rangle \\ \hat{U}\hat{a} \hat{U}^{+} \hat{U} & |coherent\rangle = \alpha \hat{U} \hat{U}^{+} \hat{U} & |coherent\rangle = \alpha \hat{U} & |coherent\rangle \\ \hat{b} \hat{U} & |coherent\rangle = \alpha \hat{U} & |coherent\rangle = \alpha \hat{U} & |coherent\rangle \\ \hat{b} \hat{U} & |coherent\rangle = \alpha \hat{U} & |coherent\rangle = \alpha \hat{U} & |coherent\rangle \end{split}
```

which says that $\hat{U}|coherent\rangle = |squeezed\rangle$. Thus, \hat{U} transforms a coherent state into a squeezed state.

14.2 Electron in a circular wire

We now consider a loop of thin wire in the shape of a circle of radius R as in Figure 14.1 below. A constant magnetic field perpendicular to the plane of the loop produces a magnetic flux passing through the loop. Imagine that the wire contains only one electron which is free to move. This electron has a wavefunction $\psi(\theta)$ which depends only on the angular coordinate θ . We neglect all interactions between the electron spin and the magnetic field as well as all magnetic fields produced by the electron itself.



Figure 14.1: Circular Wire Configuration

We first determine the energies and energy eigenfunctions for a nonrelativistic electron of mass m moving on this ring. In particular we want to find out how ground state energy of the electron depends on the value of the applied magnetic field in this approximation.

We have

$$\nabla \times \hat{A} = B\hat{e}_z$$
, $B = \text{constant}$ (14.39)

In cylindrical coordinates (r, θ, z) , we can choose

$$A_r = A_z = 0 , \ A_\theta = \frac{rB}{2} \to \vec{A} = \frac{rB}{2}\hat{e}_\theta \tag{14.40}$$

The Schrodinger equation for the electron is

$$\frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 \psi = E\psi \quad , \quad e < 0 \tag{14.41}$$

We then let

$$\psi = \psi' e^{\frac{ie}{\hbar c} \int \vec{A} \cdot d\vec{r}}$$
(14.42)

which should get rid of the effect of \vec{A} (equivalent to a gauge transformation). We have

$$\begin{split} \left(\vec{p} - \frac{e}{c}\vec{A}\right)\psi &= \left(\vec{p} - \frac{e}{c}\vec{A}\right)\psi'e^{\frac{ie}{\hbar c}\int_{\vec{r}}\vec{A}\cdot d\vec{r}} \\ &= \frac{\hbar}{i}\nabla\left(\psi'e^{\frac{ie}{\hbar c}\int_{\vec{r}}\vec{A}\cdot d\vec{r}}\right) - \frac{e}{c}\vec{A}\psi \\ &= e^{\frac{ie}{\hbar c}\int_{\vec{r}}\vec{A}\cdot d\vec{r}}\frac{\hbar}{i}\nabla\psi' + \frac{\hbar}{i}\nabla\left(e^{\frac{ie}{\hbar c}\int_{\vec{r}}\vec{A}\cdot d\vec{r}}\right)\psi' - \frac{e}{c}\vec{A}\psi \\ &= e^{\frac{ie}{\hbar c}\int_{\vec{r}}\vec{A}\cdot d\vec{r}}\frac{\hbar}{i}\nabla\psi' + \frac{e}{c}\vec{A}\psi - \frac{e}{c}\vec{A}\psi \\ &= e^{\frac{ie}{\hbar c}\int_{\vec{r}}\vec{A}\cdot d\vec{r}}\frac{\hbar}{i}\nabla\psi' = e^{\frac{ie}{\hbar c}\int_{\vec{r}}\vec{A}\cdot d\vec{r}}\vec{p}\psi' \end{split}$$

Similarly,

$$\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 \psi = e^{\frac{ie}{\hbar c}\int \vec{A} \cdot d\vec{r}} \vec{p}^2 \psi'$$
(14.43)

so that the Schrodinger equation becomes

$$\frac{1}{2m}\vec{p}^2\psi' = E\psi' \tag{14.44}$$

Since the electron is confined to a loop of radius R, we have

$$\psi = \psi(\theta) = \psi'(\theta)e^{\frac{ie}{\hbar c}\int\limits_{\vec{r}}\vec{A}\cdot d\vec{r}} = \psi'(\theta)e^{\frac{ie}{\hbar c}\int\limits_{\vec{r}}A_{\theta}Rd\theta} = \psi'(\theta)e^{\frac{ie}{\hbar c}A_{\theta}R\theta}$$
(14.45)

Therefore we have

$$\frac{1}{2m}\vec{p}^{2}\psi'(\theta) = -\frac{\hbar^{2}}{2mR^{2}}\frac{d^{2}\psi'(\theta)}{d\theta^{2}} = E\psi'(\theta) = \frac{\hbar^{2}}{2mR^{2}}C_{1}^{2}\psi'(\theta)$$
(14.46)

which has the solution

$$\psi'(\theta) = e^{iC_1\theta} \to \psi(\theta) = e^{iC_1\theta} e^{\frac{ie}{\hbar c}A_\theta R\theta} = e^{i\left(C_1 + \frac{eBR^2}{2\hbar c}\right)\theta}$$
(14.47)

Now imposing single-valuedness, we have

$$\psi(\theta) = \psi(\theta + 2\pi) \tag{14.48}$$

$$e^{i\left(C_1 + \frac{eBR^2}{2hc}\right)\theta} = e^{i\left(C_1 + \frac{eBR^2}{2hc}\right)\theta} e^{2\pi i\left(C_1 + \frac{eBR^2}{2hc}\right)}$$
(14.49)

which says that

$$C_1 + \frac{eBR^2}{2\hbar c} = n = 0, \pm 1, \pm 2, \dots$$
(14.50)

or

$$C_1 = n - \frac{eBR^2}{2\hbar c} \to E_n = \frac{\hbar^2}{2mR^2} \left(n - \frac{eBR^2}{2\hbar c}\right)^2$$
 (14.51)

If we define $\phi_0 = -\hbar c/e$ = unit of flux, and remembering that the flux through the loop is $\phi = \pi R^2 B$ we have

$$E_n = \frac{\hbar^2}{2mR^2} \left(n + \frac{\phi}{\phi_0} \right)^2 \tag{14.52}$$

which says that the dependence of E_n on the external magnetic field B or flux ϕ is parabolic. A plot is shown in Figure 14.2 below.



Figure 14.2: E_n versus B

Since n is an integer, the ground state energy ${\cal E}_g$ is given by

$$E_g = \frac{\hbar^2}{2mR^2} \left(n^* - \frac{eBR^2}{2\hbar c} \right)^2$$
(14.53)

where n^* is the integer nearest to $eBR^2/2\hbar c$ or near

$$\frac{\phi}{\phi_0} = \frac{e\phi}{c\hbar} < 0 \tag{14.54}$$

Note that $n^* < 0$ since e < 0.

Now imagine that we start with the wire in its ground state in the presence of a magnetic flux ϕ . If the magnetic field is turned off determine the current in the loop. Assume that $R = 2 \ cm$ and $\phi = 0.6 \ gauss - cm^2$.

Suppose that we start with a state E_n which is the ground state. n will remain the same when the magnetic field is turned off. Therefore, $\psi(\theta) = Ce^{in\theta}$ and the electric current is

$$\vec{J} = \frac{e\hbar}{2mi} \left(\psi^* \nabla \psi - \psi \nabla \psi^*\right) \tag{14.55}$$

which follows from

$$\nabla \cdot \vec{J} + \frac{\partial}{\partial t} \left| \psi \right|^2 = 0 \tag{14.56}$$

We then get

$$\vec{J} = \frac{e\hbar}{2mi}(in)\frac{2}{R}\psi^*\psi\hat{e}_{\theta} = \frac{ne\hbar}{mR}\psi^*\psi\hat{e}_{\theta}$$
(14.57)

Now, if S = the cross-section area of the thin wire, the normalization constant is

$$\int \psi^* \psi d\ell dS = 2\pi R |C|^2 S = 1 \to |C|^2 = \frac{1}{2\pi RS}$$
(14.58)

Then,

$$I = \text{ current } = \int \vec{J} \cdot d\vec{S} = \frac{ne\hbar}{mR} |C|^2 S = \frac{ne\hbar}{2\pi mR^2}$$
(14.59)

where we have assumed that \vec{J} is constant throughout the thin wire.

Since the electron is initially in the ground state, this implies that E_n is the minimum energy and we have

$$n = \text{greatest integer not greater than } \frac{\varphi}{\varphi_0} = \frac{e\varphi}{c\hbar}$$
 (14.60)

or

greatest integer not greater than
$$\frac{\varphi}{\varphi_0} - 1$$
 (14.61)

For a macroscopic system we have $n \gg 1$ and we can use

$$n \approx \frac{e\varphi}{c\hbar} \rightarrow I = \frac{ne\hbar}{2\pi mR^2} \approx \frac{e^2\varphi}{4\pi mcR^2}$$
 (14.62)

For $R = 2 \ cm$ and $\phi = 0.6 \ gauss - cm^2$ we have (using SI units)

$$I = \frac{(1.6 \times 10^{-19})^2 (0.6 \times 10^{-4}) \times 10^{-4}}{4\pi^2 (2 \times 10^{-2})^2 (0.9 \times 10^{-30})} = 1.1 \times 10^{-14} \, amp \tag{14.63}$$

14.3 Spin-Orbit Coupling in Complex Atoms

Spin-orbit coupling is strictly an internal effect arising from the interaction between the electron spin and the effective magnetic field due to the apparent nuclear motion. In analogy with the one-electron atom, we can write for the N-electron atom

$$\hat{H}_{so} = \sum_{i=1}^{N} \xi_i(\vec{r}_i) \vec{L}_i \cdot \vec{S}_i$$
(14.64)

where $\xi_i(\vec{r}_i)$ is defined in a manner similar to the one-electron case, assuming an effective potential field can be defined for each electron.

For the case of weak spin-orbit, let us use both classical and quantum mechanical arguments to determine the first-order correction to the energy.

Classical Argument:

Vector Model for Combining Angular Momentum: The $\vec{L} \cdot \vec{S}$ interaction causes \vec{L} and \vec{S} to exert torques on each other via their magnetic moments. This means that neither of these quantities are independently constants of the motion.

However, if $\vec{\tau}_{external} = 0$, then J^2 is a constant of the motion, where $\vec{J} = \vec{L} + \vec{S}$.

In this model, there exist two extreme orientations of these vectors for a single electron as shown in Figure 14.3 below.



Figure 14.3: Extreme Orientations

and as shown in Figure 14.4 below the \vec{L} and \vec{S} vectors precess about the vector $\vec{J} = \vec{L} + \vec{S}$ at the same angular velocity.



Figure 14.4: Precessing Vectors

The quantum conditions now apply to J^2 and J_z instead of L^2 , L_z and S^2 and S_z separately. This means that we define the state $|J, M_J\rangle$ such that

$$\hat{J}^2 |J, M_J\rangle = J(J+1)\hbar^2 |J, M_J\rangle$$
(14.65)

$$\hat{J}_z |J, M_J\rangle = M_J \hbar |J, M_J\rangle \tag{14.66}$$

where $J = |L + S|, |L + S| - 1, \dots, |L - S|$ and each J value has $2J + 1 M_J$ values.

Now consider the interaction term of the form $\sum_{i} \vec{L}_{i} \cdot \vec{S}_{i}$. In this model

each \vec{L}_i precesses rapidly about \vec{L} each \vec{S}_i precesses rapidly about \vec{S}

This means that on the average

$$\vec{L}_i = \alpha_i \vec{L} \quad , \quad \vec{S}_i = \beta_i \vec{S} \tag{14.67}$$

so that

$$\sum_{i} \vec{L}_{i} \cdot \vec{S}_{i} = \gamma \vec{L} \cdot \vec{S} \quad , \quad \gamma = \sum_{i} \alpha_{i} \beta_{i}$$
(14.68)

This means that (effectively)

$$\hat{H}_{so} = \gamma \vec{L} \cdot \vec{S} = \frac{\gamma}{2} \left(\vec{J}^2 - \vec{L}^2 - \vec{S}^2 \right)$$
(14.69)

as we assumed.

More formally (using the Wigner-Eckart theorem) we have

$$\langle LSJM | \hat{H}_{so} | LSJM \rangle = \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M'_S = M'_L + M'_S} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M'_S = M'_L + M'_S} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$= \sum_{\substack{M_L, M_S, M'_L + M'_S \\ M_L + M'_S = M'_L + M'_S} C^$$

where the last step involves two uses of the Wigner-Eckart theorem. We then have

$$\langle LSJM | \hat{H}_{so} | LSJM \rangle = \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$\times \sum_i \xi_i(r) \alpha_i \beta_i \langle LSM'_LM'_S | \vec{L} \cdot \vec{S} | LSM_LM_S \rangle$$

$$= \sum_{\substack{M_L, M_S, M'_L, M'_S \\ M_L + M_S = M'_L + M'_S}} C^* (LSM'_LM'_S) C(LSM_LM_S)$$

$$\times \langle LSM'_LM'_S | \gamma \vec{L} \cdot \vec{S} | LSM_LM_S \rangle$$

$$= \langle LSJM | \gamma \vec{L} \cdot \vec{S} | LSJM \rangle$$

$$(14.71)$$

so that effectively, \hat{H}_{so} = $\gamma \vec{L} \cdot \vec{S}.$

We also note that since

$$\hat{H}_{so} = \gamma \vec{L} \cdot \vec{S} \to E(LSJ) = A(LS) \left(\frac{J(J+1) - L(L+1) - S(S+1)}{2} \right) \quad (14.72)$$

so that

$$E(L, S, J) - E(L, S, J - 1) = A(LS) \left(\frac{J(J+1) - L(L+1) - S(S+1)}{2} \right)$$
$$- A(LS) \left(\frac{(J-1)(J) - L(L+1) - S(S+1)}{2} \right)$$
$$= \frac{A(LS)}{2} \left(J^2 + J - J^2 + J \right) = A(LS)J \qquad (14.73)$$

which is called the Lande interval rule.

14.4 Zeeman Effect in Complex Atoms

The electronic spin and orbital angular momenta in a complex atom give rise to a magnetic moment that we can write, by analogy with the one-electron atom, as

$$\vec{M} = \sum_{i=1}^{N} \vec{M}_i = -\frac{\beta}{\hbar} \sum_{i=1}^{N} \left(\vec{L}_i + 2\vec{S}_i \right)$$
(14.74)

In an external magnetic field $\vec{B} = B_z \hat{z}$, the total Hamiltonian becomes $\hat{H} = \hat{H}_0 + \hat{H}_{so} + \hat{H}_B$, where the term containing B is

$$\hat{H}_B = -\vec{M} \cdot \vec{B} = -M_z B_z \tag{14.75}$$

Let us now use classical precession arguments to derive an approximate operator expression for \hat{M}_z . We will assume both a weak spin-orbit interaction and a weak magnetic field interaction, but take the spin-orbit interaction to be dominant. Remember, in the case of weak spin-orbit interaction and a weak magnetic field, we can use the precession picture of the section 14.3. The same type of vector diagrams can be used to deal with summations like

$$\sum_{i} \vec{L}_{i} \cdot \vec{L} \quad and \quad \sum_{i} \vec{S}_{i} \cdot \vec{S} \tag{14.76}$$

By vector addition we have $\vec{J} = \vec{L} + \vec{S}$ with both \vec{L} and \vec{S} precessing rapidly about \vec{J} . Also by vector addition we have

$$\vec{\mu} = \vec{\mu}_L + \vec{\mu}_S = g_L \vec{L} + g_S \vec{S} = \frac{e}{2mc} (\vec{L} + 2\vec{S})$$
(14.77)

Clearly, $\vec{\mu}$ is not parallel to \vec{J} since

$$g_S = \frac{e}{mc} = 2g_L \tag{14.78}$$

In addition, $\vec{\mu}$ is precessing rapidly about $\vec{J}.$ Therefore,

$$\mu_{effective} = \vec{\mu} \cdot \frac{\vec{J}}{J} = -\frac{\mu_B}{\hbar} \frac{(\vec{L} + 2\vec{S}) \cdot \vec{J}}{J} = -\frac{\mu_B}{\hbar} \frac{(\vec{L} + 2\vec{S}) \cdot (\vec{L} + \vec{S})}{J}$$
$$= -\frac{\mu_B}{\hbar} \frac{(L^2 + 2S^2 + 3\vec{L} \cdot \vec{S})}{J} = -\frac{\mu_B}{\hbar} \frac{(L^2 + 2S^2 + \frac{3}{2}(J^2 - L^2 - S^2))}{J}$$
$$= -\frac{\mu_B}{\hbar} J \frac{(3J^2 - L^2 + S^2)}{2J^2} = -\frac{\mu_B}{\hbar} J \left(1 + \frac{J^2 - L^2 + S^2}{2J^2}\right)$$
(14.79)

or

$$\vec{\mu}_{effective} = -\frac{\mu_B}{\hbar} \vec{J} \left(1 + \frac{J^2 - L^2 + S^2}{2J^2} \right)$$
(14.80)

Now we use the Wigner-Eckert theorem.

14.4.1 Method #1: Plausibility Derivation

We have

$$H = -\vec{\mu} \cdot \vec{B} \tag{14.81}$$

 $\quad \text{and} \quad$

$$\vec{\mu} = \frac{e}{2mc}(\vec{L} + 2\vec{S}) = \frac{e}{2mc}(\vec{J} + \vec{S}) = G\vec{J}$$
(14.82)

by the Wigner-Eckart theorem. Therefore,

$$G\vec{J} \cdot \vec{J} = \frac{e}{2mc} (\vec{J} \cdot \vec{J} + \vec{S} \cdot \vec{J}) \rightarrow G = \frac{e}{2mc} \frac{\vec{J} \cdot \vec{J} + \vec{S} \cdot \vec{J}}{\vec{J} \cdot \vec{J}}$$
$$= \frac{e}{2mc} \frac{J(J+1) + \frac{\vec{J} \cdot \vec{J} + \vec{S} \cdot \vec{S} - \vec{L} \cdot \vec{L}}{J(J+1)}}{J(J+1)}$$
$$= \frac{e}{2mc} \left[1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \right]$$
(14.83)

14.4.2 Method #2: Full Formal Derivation

The Zeeman effect Hamiltonian is given by

$$H_{zeeman} = \frac{eB}{2mc} \left(\sum_{i} L_{iz} + 2\sum_{i} S_{iz} \right) = \frac{eB}{2mc} \left(L_z + 2S_z \right)$$
(14.84)

Therefore we need to evaluate the matrix element

$$\langle LSJM | (L_z + 2S_z) | LSJM \rangle$$

$$= \langle LSJM | J_z | LSJM \rangle + \langle LSJM | S_z | LSJM \rangle$$

$$= M\hbar + \langle LSJ ||S|| LSJ \rangle \langle JM | J_z | JM \rangle$$

$$= M\hbar (1 + \langle LSJ ||S|| LSJ \rangle)$$
(14.85)

Now

$$\langle LSJM | \vec{S} \cdot \vec{J} | LSJM \rangle = \langle LSJ ||S|| LSJ \rangle \langle LSJM | \vec{J} \cdot \vec{J} | LSJM \rangle$$

= $J(J+1)\hbar^2 \langle LSJ ||S|| LSJ \rangle$ (14.86)

or

$$\langle LSJ \| S \| LSJ \rangle = \frac{\langle LSJM | \vec{S} \cdot \vec{J} | LSJM \rangle}{J(J+1)\hbar^2}$$
(14.87)

But we have

$$\langle LSJM | \vec{S} \cdot \vec{J} | LSJM \rangle = \frac{1}{2} \langle LSJM | (J^2 + S^2 - L^2) | LSJM \rangle$$

= $\frac{\hbar^2}{2} (J(J+1) + S(S+1) - L(L+1))$ (14.88)

Putting it all together

$$\langle LSJ ||S|| LSJ \rangle = \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$
(14.89)

so that

$$\langle LSJM | (L_z + 2S_z) | LSJM \rangle = M\hbar (1 + \langle LSJ ||S|| LSJ \rangle)$$

= $M\hbar \left(1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \right)$
(14.90)

Therefore, the first-order correction to the energy level E(L, S, J) due to the perturbation \hat{H}_B is

$$\langle H_{zeeman} \rangle = \frac{eB}{2mc} M\hbar \left(1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \right)$$

= $\mu_0 Mg(LSJ)$ (14.91)

where

$$g(LSJ) = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$
(14.92)

is the so-called Lande g-factor.

14.5 Neutron Interferometry

In the late 1970s several neutron interference experiments which are of fundamental importance in quantum mechanics and which settled debates started in 1930s, were carried out by Overhauser and collaborators.

In this section we investigate the effects on a neutron interference pattern of the

gravitational field.

We mentioned some aspects of this type of experiment in Chapter 16. Here we go into more detail.

We consider an interferometer made of three parallel equally spaced crystalline silicon strips as shown in Figure 14.5 below.



Figure 14.5: Experimental Setup

The incident neutron beam is assumed to be monochromatic. C_2 and C_3 are neutron counters.

For a particular value of the angle of incidence $\theta,$ called the Bragg angle, a plane wave

$$\psi_{inc} = e^{i(\vec{p}\cdot\vec{r}-Et)/\hbar} \tag{14.93}$$

where E is the energy of the neutrons and \vec{P} their momentum, is split by the crystal into two outgoing waves which are symmetric with respect to the direction perpendicular to the crystal, as shown in Figure 14.6 below.



Figure 14.6: Splitting Waves

The transmitted wave and the reflected wave have complex amplitudes which can be written respectively as

$$\alpha = \cos \chi$$
, $\beta = i \sin \chi$ χ real (14.94)

so that

$$\psi_I = \alpha e^{i(\vec{p}\cdot\vec{r}-Et)/\hbar}$$
, $\psi_{II} = \beta e^{i(\vec{p}'\cdot\vec{r}-Et)/\hbar}$ (14.95)

where $|\vec{p}| = |\vec{p}'|$ since the neutrons scatter elastically on the nuclei of the crystal. The transmission and reflection coefficients are

$$T = |\alpha|^2$$
, $R = |\beta|^2$ with $T + R = 1$ (14.96)

In this interferometer setup the incident neutron beam is horizontal. It is split by the interferometer into a set of beams, two of which recombine and interfere at point D. The detectors C_2 and C_3 count the outgoing neutron fluxes. The neutron beam velocity corresponds to a de Broglie wavelength $\lambda = 1.445$ and the neutron mass is $M = 1.675 \times 10^{-27} kg$.

For calculational simplicity we are using monochromatic plane waves to represent the neutron beams; they are, however, quasi-monochromatic with finite extension in directions transverse to the beams.

14.5.1 Neutron Interferences

The measured neutron fluxes are proportional to the intensities of the waves that reach the counters. We define the intensity of the incoming wave to be 1 (units are arbitrary). For C_2 the beams $ABDC_2$ and $ACDC_2$ interfere. Omitting the propagation factors, at C_2 we have the amplitude

$$A_2 = \alpha^2 \beta + \beta^3 = \beta (\alpha^2 + \beta^2) \tag{14.97}$$

Similarly, for $ABDC_2$ and $ACDC_3$,

$$A_3 = 2\alpha\beta^2 \tag{14.98}$$

The intensities at the two counters are then

$$I_2 = R - 4R^2T \quad , \quad I_3 = 4R^2T \tag{14.99}$$

Suppose that we create a phase shift δ of the wave propagating along AC, i.e., in C the wave function is multiplied by $e^{i\delta}$.

The new amplitudes at the detectors are

$$A_{2} = \alpha^{2} \beta e^{i\delta} + \beta^{3} = \beta (\alpha^{2} e^{i\delta} + \beta^{2}) \quad , \quad A_{3} = \alpha \beta^{2} (1 + e^{i\delta})$$
(14.100)

and the new intensities become

$$I_2 = R - 2R^2T(1 + \cos\delta)$$
, $I_3 = 2R^2T(1 + \cos\delta)$ (14.101)

Note that $I_2 + I_3$ does not depend on the phase shift δ . This is because of the conservation of the total number of particles arriving at D.

The phase difference δ between the beams ACD and ABD is created by rotating the interferometer by an angle φ around the direction of the incident beam as shown in Figure 14.7 (on the left)below.



Figure 14.7: Geometrical Considerations

Now let d be the distance between the silicon strips (we neglect their thickness in this discussion). We also define L as the side of ABCD and H as its height as shown in Figure 14.7 (on the right) above. We then have(simple geometry) that

$$L = \frac{d}{\cos \theta}$$
, $H = 2d \sin \theta$ $\theta = \text{Bragg angle}$ (14.102)

Experimentally, the values of d and θ are $d = 3.6 \, cm$ and $\theta = 22.1 \,^{\circ}$.

For an angle φ we define the gravitational potential V to be V = 0 along AC and $V = V_0$ along BD.

Since there is no recoil energy of the silicon atoms to be taken into account, the neutron total energy (kinetic + potential) is a constant of the motion in all of the process. The energies are given by

$$E_{AC} = \frac{p^2}{2M} = E_{BD} = \frac{(p - \Delta p)^2}{2M} + MgH\sin\phi \qquad (14.103)$$

$$\Delta p \approx \frac{M^2 g H \sin \phi}{p} \tag{14.104}$$

where Δp is the difference in the neutron momentum.

The velocity $\sqrt{2gH}$ is of order 0.5 m/s and the neutron velocity is

$$v = \frac{h}{M\lambda} \approx 2700 \ m/s \tag{14.105}$$

The change in the velocity Δv is therefore very small, i.e.,

$$\Delta v = \frac{gH}{v} \approx 2 \times 10^{-4} \ m/s \quad \text{for} \quad \phi = \frac{\pi}{2} \tag{14.106}$$

Now the gravitational potential varies in exactly the same way along AB and CD. The neutron state in both cases is a plane wave with momentum $p = h/\lambda$ just before A or C. The same Schrodinger equation is used to determine the wave function at the end of the segments. This implies that the phases accumulated along the two segments AB and CD are equal.

When comparing segments AC and BD, the previous reasoning does not apply, since the initial state of the neutron is not the same for the two segments. The initial state is $e^{ipz/\hbar}$ for AC and $e^{i(p-\Delta p)z/\hbar}$ for BD. After traveling over a distance $L = \overline{AC} - \overline{BD}$, the phase difference between the two paths is

$$\delta = \frac{L\Delta p}{\hbar} = \frac{M^2 g \lambda d^2}{\pi \hbar^2} \tan \theta \sin \phi \qquad (14.107)$$

The variation with φ of the experimentally measured intensity I_2 in the counter C_2 is shown schematically in Figure 14.8 below (the data does not display a minimum exactly at $\varphi = 0$ because of calibration difficulties).



Figure 14.8: Variation of Intensity with φ

From the previous result, we have

$$\delta_2 - \delta_1 = Ag(\sin \phi_2 - \sin \phi_1)$$
 (14.108)

where

$$A = \frac{M^2 \lambda d^2}{\pi \hbar^2} \tan \theta \tag{14.109}$$

Therefore,

$$g = \frac{\delta_2 - \delta_1}{A(\sin \phi_2 - \sin \phi_1)}$$
(14.110)

In the actual data there are 9 oscillations, i.e., $\delta_2 - \delta_1 = 18\pi$ between $\varphi_1 = -32^{\circ}$ and $\varphi_2 = +24^{\circ}$, which gives $g = 9.8 m/s^2$. This clearly shows that the neutron interference effects are directly the result of the difference in the gravitational potential along two arms of the interferometer.

14.6 The Penning Trap

A Penning trap allows one to confine electrons in a finite spatial region and then allow the accurate measurement of various properties. It involves the superposition of a uniform magnetic field \vec{B} directed along the z-axis and a quadrupole electric field which derives from an electrostatic potential of the form

$$\Phi = \mathcal{K}(2z^2 - x^2 - y^2) \tag{14.111}$$

where K is a positive constant.

An electron of charge -q(q > 0) and mass m is placed in such a device. We denote its spin operator by \vec{S} and its momentum operator by \vec{p} . The Hamiltonian of the electron in the above superposition of fields is

$$\hat{H} = \frac{1}{2m} \left(\vec{p} + q\vec{A}(\vec{r}) \right)^2 + V(\vec{r}) + (1+a) \frac{q}{m} \vec{S} \cdot \vec{B}$$
(14.112)

$$V(\vec{r}) = \Phi = m\omega_0^2 (2\hat{z}^2 - \hat{x}^2 - \hat{y}^2)/4$$
(14.113)

= electrostatic potential energy (14.114)

$$\vec{A}(\vec{r}) = \vec{B} \times \vec{r}/2 \tag{14.115}$$

= vector potential (14.116)

The constant $a\approx 1.16\times 10^{-3}$ is the gyromagnetic anomaly of the electron magnetic moment.

14.6.1 Motion of an Electron in a Penning Trap

We set $\omega_c = qB/m$, where B is the magnitude of the magnetic field, and we assume that this cyclotron frequency ω_c is much larger than ω_0 .

We note that
$$\vec{p} \cdot \vec{A}(\vec{r}) = \vec{A}(\vec{r}) \cdot \vec{p} = \vec{L} \cdot \vec{B}/2 = \hat{L}_z B/2$$
 and $\vec{A}^2 = B^2(x^2 + y^2)/4$. We

then get

$$\hat{H} = \hat{H}_z + \hat{H}_t + \hat{H}_s$$
(14.117)

$$\hat{H}_z = \frac{\hat{p}_z^2}{2m} + \frac{1}{2}m\omega_0^2 \hat{z}^2 \tag{14.118}$$

$$\hat{H}_t = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\Omega^2(\hat{x}^2 + \hat{y}^2) + \frac{1}{2}\omega_c\hat{L}_z$$
(14.119)

$$\hat{H}_s = (1+a)\omega_c \hat{S}_z \tag{14.120}$$

with $\Omega^2 = (\omega_c^2 - 2\omega_0^2)/4 \Rightarrow \Omega \simeq \omega_c/2 - \omega_0^2/2\omega_c$ and \vec{L} is the orbital angular momentum of the electron.

The eigenstates of \hat{H}_s are the eigenstates of \hat{S}_z , $|\pm\rangle$ with energy eigenvalues

$$\pm (1+a)\hbar\omega_c/2 = \pm\hbar\omega_s \quad , \quad \omega_s = (1+a)\omega_c/2 \tag{14.121}$$

where we have used

$$\hat{S}_{z}\left|\pm\right\rangle = \pm\hbar/2\left|\pm\right\rangle \tag{14.122}$$

Since \hat{H}_z , \hat{H}_t and \hat{H}_s act on different variables, they must commute. An eigenbasis of \hat{H} can be constructed using the eigenstates $\varphi(z)$, $\psi(x,y)$ and $|\sigma\rangle$ of \hat{H}_z , \hat{H}_t and \hat{H}_s , respectively. The corresponding eigenvalues are the sum of the individual eigenvalues.

In order to calculate the motion along the z-axis, we introduce the creation and annihilation operators

$$\hat{a}_z = \frac{1}{\sqrt{2}} \left(\alpha \hat{z} + \frac{i}{\alpha \hbar} \hat{p}_z \right) \quad , \quad \hat{a}_z^+ = \frac{1}{\sqrt{2}} \left(\alpha \hat{z} - \frac{i}{\alpha \hbar} \hat{p}_z \right) \quad , \quad \alpha = \sqrt{m \hbar \omega_0}$$

We then have

$$\begin{bmatrix} \hat{a}_{z}, \hat{a}_{z}^{+} \end{bmatrix} = \frac{1}{2} \left(\alpha^{2} \begin{bmatrix} \hat{z}, \hat{z} \end{bmatrix} + \frac{i}{\hbar} \begin{bmatrix} \hat{p}_{z}, \hat{z} \end{bmatrix} - \frac{i}{\hbar} \begin{bmatrix} \hat{z}, \hat{p}_{z} \end{bmatrix} - \frac{1}{\alpha^{2} \hbar^{2}} \begin{bmatrix} \hat{p}_{z}, \hat{p}_{z} \end{bmatrix} \right)$$

$$= \frac{1}{2} \left(+ \frac{i}{\hbar} \begin{bmatrix} -i\hbar \end{bmatrix} - \frac{i}{\hbar} \begin{bmatrix} i\hbar \end{bmatrix} \right) = 1$$
(14.123)

Thus, we have the same mathematical system as the harmonic oscillator so that

$$\hat{H}_z = \hbar \omega_0 (\hat{N}_z + 1/2) \quad , \quad \hat{N}_z = \hat{a}_z^+ \hat{a}_z$$
 (14.124)

$$\hat{N}_z |N_z\rangle = N_z |N_z\rangle$$
 , $N_z = 0, 1, 2, 3, \dots$ (14.125)

$$\hat{H}_z |N_z\rangle = E_{N_z} |N_z\rangle \quad , \quad E_{N_z} = \hbar\omega_0 (N_z + 1/2)$$
 (14.126)

14.6.2 The Transverse Motion

We now investigate the x - y motion governed by the Hamiltonian \hat{H}_t . If we define the right- and left-circular creation and annihilation operators

$$\hat{a}_{r} = \frac{1}{2} \left(\beta (\hat{x} - i\hat{y}) + \frac{i}{\beta \hbar} (\hat{p}_{x} - i\hat{p}_{y}) \right)$$
(14.127)

$$\hat{a}_{l} = \frac{1}{2} \left(\beta(\hat{x} + i\hat{y}) + \frac{i}{\beta\hbar} (\hat{p}_{x} + i\hat{p}_{y}) \right)$$
(14.128)

where β is a real constant, then we can show (in same way as above) that

$$[\hat{a}_r, \hat{a}_r^+] = 1 = [\hat{a}_l, \hat{a}_l^+] \quad , \quad [\hat{a}_r, \hat{a}_l] = 0 = [\hat{a}_r, \hat{a}_l^+]$$
(14.129)

Defining

$$\hat{N}_r = \hat{a}_r^+ \hat{a}_r \quad , \quad \hat{N}_l = \hat{a}_l^+ \hat{a}_l$$
 (14.130)

we have

$$\hat{N}_r = \hat{a}_r^+ \hat{a}_r = \frac{1}{4} \left(\beta^2 (x^2 + y^2) + \frac{1}{\beta^2 \hbar^2} (p_x^2 + p_y^2) - 2 + \frac{2L_z}{\hbar} \right)$$
(14.131)

$$\hat{N}_{l} = \hat{a}_{l}^{\dagger} \hat{a}_{l} = \frac{1}{4} \left(\beta^{2} (x^{2} + y^{2}) + \frac{1}{\beta^{2} \hbar^{2}} (p_{x}^{2} + p_{y}^{2}) - 2 - \frac{2L_{z}}{\hbar} \right)$$
(14.132)

and thus

$$\hat{L}_{z} = \hat{x}\hat{p}_{y} - \hat{y}\hat{p}_{x} = \hbar(\hat{N}_{r} - \hat{N}_{l})$$
(14.133)

 $\quad \text{and} \quad$

$$\hat{N}_r + \hat{N}_l = \frac{1}{2} \left(\beta^2 (x^2 + y^2) + \frac{1}{\beta^2 \hbar^2} (p_x^2 + p_y^2) \right) - 1$$
(14.134)

If we define $\beta^2 = m\Omega/\hbar$ we then have

$$\hat{H}_{t} = \hbar \Omega (\hat{N}_{r} + \hat{N}_{l} + 1) + \frac{\hbar \omega_{c}}{2} (\hat{N}_{r} - \hat{N}_{l})$$
(14.135)

 or

$$\hat{H}_t = \hbar \omega_c' (\hat{N}_r + 1/2) - \hbar \omega_m (\hat{N}_l + 1/2)$$
(14.136)

where

$$\omega_c' = \frac{\omega_c}{2} + \Omega = \frac{1}{2} \left(\omega_c + \sqrt{\omega_c^2 - 2\omega_0^2} \right) \simeq \omega_c \tag{14.137}$$

$$\omega_m = \frac{\omega_c}{2} - \Omega = \frac{1}{2} \left(\omega_c - \sqrt{\omega_c^2 - 2\omega_0^2} \right) \simeq \frac{\omega_0^2}{2\omega_c} \ll \omega_c \tag{14.138}$$

Since this is just the difference of two oscillators we have the energy eigenvalues

$$E_{cm} = \hbar \omega_c'(N_c + 1/2) - \hbar \omega_m (N_m + 1/2)$$
(14.139)

We also have from earlier

$$\pm (1+a)\hbar\omega_c/2 = \pm\hbar\omega_s$$
 , $\omega_s = (1+a)\omega_c/2$ (14.140)

Thus, the energy eigenvalues of \hat{H} are

$$E = \hbar\omega_0 (N_z + 1/2) + \hbar\omega_c' (N_c + 1/2) - \hbar\omega_m (N_m + 1/2) + \sigma\hbar\omega_s \qquad (14.141)$$

where N_z , N_c and N_m are integers ≥ 0 and $\sigma = \pm 1$.

Note that the magnetron motion E_m corresponds to an inverted harmonic oscillator, so that its spectrum has no mower bound in the harmonic approximation used in the example. Consequently, when the system is coupled to a heat bath and relaxes towards thermal equilibrium, it should cascade down the ladder of levels of the magnetron motion, thus increasing the size of the orbit of the trapped particle in the xy-plane. Fortunately, the characteristic time corresponding to the decay of the system in this way is very long, and the electron can be confined around the center of the trap for a long time.

14.6.3 Measurement of Electron Anomalous Magnetic Moment

The electric quadrupole field is such that $\hbar\omega_0 = 2.58 \times 10^{-7} eV$. The magnetic field is B = 5.87 T. The system is placed in liquid helium at 4.2 K. We then have (using $q\hbar/2m = 5.79 \times 10^{-5} eV$)

$$\hbar\omega_c = 6.8 \times 10^{-4} eV \sim \hbar\omega'_c$$
$$\hbar\omega_m = 4.9 \times 10^{-11} eV$$

In liquid helium, $kT = 3.5 \times 10^{-4} eV$ and the longitudinal and magnetron level spacings are much smaller than the thermal fluctuations. Thus, a classical description of these two motions is appropriate. In contrast, a few quanta of oscillation are thermal excited for the cyclotron motion since $kT \leq \hbar\omega_c$. Now, the electron anomaly is $a \approx 0.00116$. Therefore we can draw the relative position of the four energy levels

$$N_z = 0; \ N_m = 0; \ N_c = 0, 1 \ and \ \sigma = \pm 1$$
 (14.142)

The level configuration is shown in Figure 14.9 below.



Figure 14.9: Energy Levels

The splitting ΔE between the level $N_c = 0, \sigma = +1$ and the level $N_c = 1, \sigma = -1$ is proportional to the anomaly a. We have $\Delta E = a\hbar\omega_c = 5 \times 10^{-7} eV$, where we have neglected the difference between ω_c and ω'_c which is $\approx 7.9 \times 10^{-11} eV$. The splitting corresponds to a frequency $\nu = \Delta E/\hbar = 191 MHz$.

14.7 Schrodinger's Cat

We first just describe a simple version.

Suppose that a cat within a closed box would be killed by a $|\uparrow\rangle$ particle but not by a $|\downarrow\rangle$ particle. Now consider the effect of the state $|\uparrow\rangle + Ket\downarrow$, which can easily be produced by a properly oriented Stern-Gerlach device.

Suppose that a particle in the state $|\uparrow\rangle + Ket\downarrow$ hits the cat and that the state of the (spin + cat) makes a transition to

$$|\uparrow\rangle |dead \, cat\rangle + |\downarrow\rangle |living \, cat\rangle \tag{14.143}$$

which is a *pure state*.

When is it decided whether the cat is alive or dead?

Just when the observer opens the cat's box?

An objective statement independent of the conscious mind of the observer would be impossible.

What is the consequence of including the observer herself in the quantum mechanical description?

According to the point of view presented, the cat(together with the mechanism for killing the cat, which was not mentioned above) is linked to other macroscopic objects. These are influenced differently in the two final states so that their respective wave functions do not overlap. For everything that follows, the macroscopic consequences are not recorded; the trace is taken over them. The final state of the cat is described by a mixture of states corresponding to a dead cat and a living cat: the cat is *either* dead *or* living and not in a pure state

$$|dead cat\rangle + |living cat\rangle$$
 (14.144)

which would include both possibilities.

14.7.1 Schrodinger's Cat - a more detailed presentation

The superposition principle states that if $|\varphi_a\rangle$ and $|\varphi_b\rangle$ are two possible states of a quantum system, the quantum superposition

$$\frac{1}{\sqrt{2}}\left(|\varphi_a\rangle + |\varphi_b\rangle\right) \tag{14.145}$$

is also an allowed state for this system. This principle is essential in explaining quantum interference phenomena. However, when it is applied to *large* or *macroscopic* objects, it leads to paradoxical situations where a system can be in a superposition of states which is classical self-contradictory.

The most famous example is Schrodinger's *cat paradox* where the cat is in a superposition of the *dead* and *alive* states. The purpose of this discussion is to show that such superposition of macroscopic states are not detectable in practice. They are extremely fragile, and very weak coupling to the environment suffices to destroy the quantum superposition of the two states $|\varphi_a\rangle$ and $|\varphi_b\rangle$.

The Quasi-Classical States of a Harmonic Oscillator

We consider the high energy excitations of a one-dimensional harmonic oscillator or mass m and frequency ω . The Hamiltonian is written

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 \tag{14.146}$$

We denote the eigenstates of \hat{H} by $\{|n\rangle\}$ where the energy eigenvalues are given by

$$\hat{H}|n\rangle = E_n|n\rangle = \hbar\omega(n+1/2)|n\rangle$$
(14.147)

Preliminaries

We introduce the operators

$$\hat{X} = \sqrt{m\omega/\hbar}\hat{x}$$
, $\hat{P} = \hat{p}/\sqrt{m\hbar\omega}$ (14.148)

and the annihilation and creation operators

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\hat{X} + i\hat{P} \right) \quad , \quad \hat{a}^{+} = \frac{1}{\sqrt{2}} \left(\hat{X} - i\hat{P} \right) \quad , \quad \hat{N} = \hat{a}^{+}\hat{a}$$
(14.149)

The commutator $[\hat{x}, \hat{p}] = i\hbar$ leads to the commutators $[\hat{X}, \hat{P}] = i$ and $[\hat{a}, \hat{a}^+] = 1$ and the relations

$$\hat{H} = \hbar\omega(\hat{N} + 1/2) \quad , \quad \hat{N}|n\rangle = n|n\rangle$$
 (14.150)

We also have the relations

$$\hat{P} = -i\frac{\partial}{\partial X}$$
, $\hat{X} = i\frac{\partial}{\partial P}$ (14.151)

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$
, $\hat{a}^{+}|n\rangle = \sqrt{n+1}|n+1\rangle$ (14.152)

We can use these relations to derive the ground state wave function in the position representation as follows:

$$0 = \langle X | \hat{a} | 0 \rangle = \frac{1}{\sqrt{2}} \langle X | (\hat{X} + i\hat{P}) | 0 \rangle$$

$$= \frac{1}{\sqrt{2}} X \langle X | 0 \rangle + \frac{i}{\sqrt{2}} \left(-i \frac{\partial}{\partial X} \right) \langle X | 0 \rangle$$

$$\left(X + \frac{\partial}{\partial X} \right) \langle X | 0 \rangle = 0 \rightarrow \langle X | 0 \rangle = A e^{-X^2/2} = \psi_0(X)$$

$$\psi_0(x) = A e^{-m\omega x^2/2\hbar}$$
(14.153)

Similarly, we can derive its the ground state wave function in the momentum representation as follows:

$$0 = \langle P | \hat{a} | 0 \rangle = \frac{1}{\sqrt{2}} \langle P | (\hat{X} + i\hat{P}) | 0 \rangle$$

$$= \frac{1}{\sqrt{2}} i \frac{\partial}{\partial P} \langle P | 0 \rangle + \frac{i}{\sqrt{2}} P \langle P | 0 \rangle$$

$$\left(P + \frac{\partial}{\partial P} \right) \langle P | 0 \rangle = 0 \rightarrow \langle P | 0 \rangle = A e^{-P^2/2} = \phi_0(P)$$

$$\phi_0(p) = A e^{-p^2/2m\omega\hbar}$$
(14.154)

These two wave functions are related by the Fourier transform, that is,

$$\phi_0(p) = e^{-p^2/2m\omega\hbar} \propto \int_{-\infty}^{\infty} e^{-m\omega x^2/2\hbar} e^{-ipx/\hbar} dx$$
$$\propto \int_{-\infty}^{\infty} \psi_0(x) e^{-ipx/\hbar} dx$$

The Quasi-Classical States

The eigenstates of the operator \hat{a} are called *quasi-classical* states, for reasons we will now discuss.

Since we are considering the question: what are the eigenstates of the lowering operator \hat{a} ? We can write

$$\hat{a} |\alpha\rangle = \alpha |\alpha\rangle$$
 where $\alpha = |\alpha| e^{i\phi}$ (14.155)

where $|\alpha\rangle$ is the eigenvector of \hat{a} and α is the eigenvalue, which is not necessarily real since \hat{a} is not Hermitian.

Since the vectors $|n\rangle$ are eigenvectors of a Hermitian operator, they form a

orthonormal complete set and can be used as an orthonormal basis for the vector space. We can then write

$$|\alpha\rangle = \sum_{m=0}^{\infty} b_m |m\rangle \tag{14.156}$$

where

$$\langle k \mid \alpha \rangle = \sum_{m=0}^{\infty} b_m \langle k \mid m \rangle = \sum_{m=0}^{\infty} b_m \delta_{km} = b_k$$
(14.157)

Now

$$\langle n-1 | \hat{a} | \alpha \rangle = \alpha \langle n-1 | \alpha \rangle = \alpha b_{n-1}$$
(14.158)

and using

$$\hat{a}^{+} |n-1\rangle = \sqrt{n} |n\rangle \rightarrow \langle n-1| \,\hat{a} = \sqrt{n} \, \langle n| \qquad (14.159)$$

we have

$$\langle n-1|\hat{a}|\alpha\rangle = \sqrt{n} \langle n|\alpha\rangle = \sqrt{n}b_n \qquad (14.160)$$

 or

$$b_n = \frac{\alpha}{\sqrt{n}} b_{n-1} \tag{14.161}$$

This says that

$$b_1 = \frac{\alpha}{\sqrt{1}}b_0$$
 , $b_2 = \frac{\alpha}{\sqrt{2}}b_1 = \frac{\alpha^2}{\sqrt{2!}}b_0$ (14.162)

 \mathbf{or}

$$b_n = \frac{\alpha^n}{\sqrt{n!}} b_0 \tag{14.163}$$

We thus get the final result

$$|\alpha\rangle = b_0 \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} |m\rangle \tag{14.164}$$

Let us now normalize this state (choose b_0). We have

$$\langle \alpha \mid \alpha \rangle = 1 = |b_0|^2 \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} \frac{\alpha^{*m} \alpha^k}{\sqrt{m!} \sqrt{k!}} \langle k \mid m \rangle$$

= $|b_0|^2 \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} \frac{\alpha^{*m} \alpha^k}{\sqrt{m!} \sqrt{k!}} \delta_{km} = |b_0|^2 \sum_{m=0}^{\infty} \frac{|\alpha|^2}{m!}$
= $|b_0|^2 e^{|\alpha|^2}$ (14.165)

which says that

$$b_0 = e^{-\frac{1}{2}|\alpha|^2} \tag{14.166}$$

and thus

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} |m\rangle$$
(14.167)

Now

$$\langle n \mid \alpha \rangle$$
 = probability amplitude that the system in the state
 $\mid \alpha \rangle$ will be found in the state $\mid n \rangle$

We have

$$\langle n \mid \alpha \rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} \langle n \mid m \rangle = e^{-\frac{1}{2}|\alpha|^2} \frac{\alpha^n}{\sqrt{n!}}$$
(14.168)

which then says that

$$P_n = |\langle n \mid \alpha \rangle|^2 = \frac{e^{-|\alpha|^2} |\alpha|^{2n}}{n!} = \frac{e^{-N} N^n}{n!}$$

= probability amplitude that the system in the state
 $|\alpha\rangle$ will be found in the state $|n\rangle$

where we have defined $N = |\alpha|^2$. We note that

$$\langle \alpha | \hat{a}^{\dagger} \hat{a} | \alpha \rangle = \left| \alpha^{2} \right| \langle \alpha | \alpha \rangle = \left| \alpha^{2} \right| = N = \langle \alpha | \hat{N}_{op} | \alpha \rangle$$
(14.169)

or N = the average value or expectation value of the N_{op} operator in the state $|\alpha\rangle$. This type of probability distribution is called a Poisson distribution, i.e., the state $|\alpha\rangle$ has the number states or energy eigenstates distributed in a *Poisson* manner.

Since the states $|n\rangle$ are energy eigenstates, we know their time dependence, i.e.,

$$|n,t\rangle = e^{-i\frac{E_n}{\hbar}t}|n\rangle \tag{14.170}$$

Therefore, we have for the time dependence of the state $|\alpha\rangle$

$$|\alpha, t\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} |m, t\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} e^{-i\frac{E_m}{\hbar}t} |m\rangle$$
(14.171)

This simple operation clearly indicates the fundamental importance of the energy eigenstates when used as a basis set.

If we are able to expand an arbitrary vector representing some physical system in the energy basis, then we immediately know the time dependence of that state vector and hence we know the time dependence of all the probabilities associated with the state vector and the system.

Now let us try to understand the physics contained in the $|\alpha\rangle$ state vector. In a

given energy eigenstate the expectation value of the position operator is given by

$$\begin{split} \langle n,t|\,\hat{x}\,|n,t\rangle &= \sqrt{\frac{\hbar}{2m\omega_0}}\,\langle n,t|\,(\hat{a}+\hat{a}^+)\,|n,t\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega_0}}\,\langle n|\,e^{i\frac{E_n}{\hbar}t}(\hat{a}+\hat{a}^+)e^{-i\frac{E_n}{\hbar}t}\,|n\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega_0}}\,\langle n|\,(\hat{a}+\hat{a}^+)\,|n\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega_0}}\,\langle n|\,\left(\sqrt{n}\,|n-1\rangle+\sqrt{n+1}\,|n+1\rangle\right) = 0 \end{split}$$

i.e., it is equal to zero and is a constant.

On the other hand, in the state $|\alpha\rangle$ we find

$$\langle \alpha, t | \hat{x} | \alpha, t \rangle = \sqrt{\frac{\hbar}{2m\omega_0}} \sum_m \sum_k b_m^* b_k e^{i\frac{(E_m - E_k)}{\hbar}t} \langle m | (\hat{a} + \hat{a}^+) | k \rangle$$
(14.172)

Now

$$\langle m | (\hat{a} + \hat{a}^{\dagger}) | k \rangle = \langle m | \left(\sqrt{k} | k - 1 \rangle + \sqrt{k + 1} | k + 1 \rangle \right)$$
$$= \sqrt{k} \delta_{m,k-1} + \sqrt{k + 1} \delta_{m,k+1}$$
(14.173)

Using this result we have

$$\begin{aligned} \langle \alpha, t | \, \hat{x} \, | \alpha, t \rangle &= \sqrt{\frac{\hbar}{2m\omega_0}} \left(\sum_{k=1}^{\infty} b_{k-1}^* b_k \sqrt{k} e^{i\frac{(E_{k-1}-E_k)}{\hbar}t} + \sum_{k=0}^{\infty} b_{k+1}^* b_k \sqrt{k+1} e^{i\frac{(E_{k+1}-E_k)}{\hbar}t} \right) \\ &= \sqrt{\frac{\hbar}{2m\omega_0}} \left(\sum_{k=1}^{\infty} b_{k-1}^* b_k \sqrt{k} e^{-i\omega_0 t} + \sum_{k=0}^{\infty} b_{k+1}^* b_k \sqrt{k+1} e^{i\omega_0 t} \right) \\ &= \sqrt{\frac{\hbar}{2m\omega_0}} \left(\sum_{k=0}^{\infty} b_k^* b_{k+1} \sqrt{k} e^{-i\omega_0 t} + \sum_{k=0}^{\infty} b_{k+1}^* b_k \sqrt{k+1} e^{i\omega_0 t} \right) \\ &= \sqrt{\frac{\hbar}{2m\omega_0}} b_0^2 \left(\sum_{k=0}^{\infty} \frac{\alpha^{*k} \alpha^{k+1}}{\sqrt{(k+1)!k!}} \sqrt{k} e^{-i\omega_0 t} + \sum_{k=0}^{\infty} \frac{\alpha^{*k+1} \alpha^k}{\sqrt{(k+1)!k!}} \sqrt{k+1} e^{i\omega_0 t} \right) \\ &= \sqrt{\frac{\hbar}{2m\omega_0}} b_0^2 \sum_k \frac{1}{k!} |\alpha|^{2k} \left(\alpha e^{-i\omega_0 t} + \alpha^* e^{i\omega_0 t} \right) \end{aligned} \tag{14.174}$$

Now using $\alpha = |\alpha|e^{i\varphi}$ we get

$$\langle \alpha, t | \hat{x} | \alpha, t \rangle = \sqrt{\frac{\hbar}{2m\omega_0}} b_0^2 2 |\alpha| \sum_k \frac{|\alpha|^{2k}}{k!} \operatorname{Real}(e^{i\phi} e^{-i\omega_0 t})$$
$$= 2x_0 |\alpha| \cos(\omega_0 t - \phi) (b_0^2 \sum_k \frac{|\alpha|^{2k}}{k!})$$
$$= 2x_0 |\alpha| \cos(\omega_0 t - \phi) \quad , \quad x_0 = \sqrt{\frac{\hbar}{2m\omega_0}} \tag{14.175}$$

The expectation value in the state $|\alpha\rangle$ behaves like that of a *classical oscillator*.

Before proceeding with the discussion, we will repeat the derivation using an alternate but very powerful technique.

Using the Translation Operator

In general, a displaced state $|\lambda\rangle$ is given in terms of the displacement operator (in one dimension) by

$$|\lambda\rangle = e^{-\frac{i}{\hbar}\hat{p}\lambda}|0\rangle \tag{14.176}$$

For the harmonic oscillator system

$$\hat{p} = \frac{1}{i} \sqrt{\frac{m\hbar\omega}{2}} (\hat{a} - \hat{a}^{+})$$
 (14.177)

If we choose $|0\rangle$ to be the ground state of the oscillator, then we have for the corresponding displaced ground-state

$$|\lambda\rangle = e^{\sqrt{\frac{m\omega}{2\hbar}}(\hat{a}^{\dagger} - \hat{a})\lambda} |0\rangle \tag{14.178}$$

By Glauber's theorem

$$e^{(\hat{A}+\hat{B})} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A},\hat{B}]}$$
(14.179)

we have

$$e^{\sqrt{\frac{m\omega}{2\hbar}}(\hat{a}^{+}-\hat{a})\lambda} = e^{\sqrt{\frac{m\omega}{2\hbar}}\hat{a}^{+}\lambda}e^{-\sqrt{\frac{m\omega}{2\hbar}}\hat{a}\lambda}e^{\frac{1}{2}\frac{m\omega}{2\hbar}}[\hat{a}^{+},\hat{a}]\lambda^{2}$$
$$= e^{\sqrt{\frac{m\omega}{2\hbar}}\hat{a}^{+}\lambda}e^{-\sqrt{\frac{m\omega}{2\hbar}}\hat{a}\lambda}e^{-\frac{1}{4}\frac{m\omega}{\hbar}\lambda^{2}}$$
(14.180)

and thus

$$\left|\lambda\right\rangle = e^{\sqrt{\frac{m\omega}{2\hbar}}\hat{a}^{+}\lambda} e^{-\sqrt{\frac{m\omega}{2\hbar}}\hat{a}\lambda} e^{-\frac{1}{4}\frac{m\omega}{\hbar}\lambda^{2}} \left|0\right\rangle \tag{14.181}$$

Now

$$e^{-\sqrt{\frac{m\omega}{2\hbar}}\hat{a}\lambda}\left|0\right\rangle = \left(\hat{I} + \left(-\sqrt{\frac{m\omega}{2\hbar}}\lambda\hat{a}\right) + \frac{1}{2}\left(-\sqrt{\frac{m\omega}{2\hbar}}\lambda\hat{a}\right)^2 + \dots\right)\left|0\right\rangle = \left|0\right\rangle$$

using $\hat{a} |0\rangle = 0$. Similarly, using $(\hat{a}^+)^n |0\rangle = \sqrt{n!} |n\rangle$ we have

$$e^{\sqrt{\frac{m\omega}{2\hbar}}\hat{a}^{+}\lambda}|0\rangle = \left(\hat{I} + \left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\hat{a}^{+}\right) + \frac{1}{2}\left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\hat{a}^{+}\right)^{2} + \dots\right)|0\rangle$$
$$= |0\rangle + \sqrt{\frac{m\omega}{2\hbar}}\lambda|1\rangle + \frac{1}{2}\left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\right)^{2}|2\rangle + \dots$$
$$= \sum_{n=0}^{\infty} \frac{\left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\right)^{n}}{\sqrt{n!}}|n\rangle$$
(14.182)

 \mathbf{or}

$$|\lambda\rangle = e^{-\frac{1}{4}\frac{m\omega}{\hbar}\lambda^2} \sum_{n=0}^{\infty} \frac{\left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\right)^n}{\sqrt{n!}} |n\rangle$$
(14.183)

Thus,

$$|\lambda\rangle = \sum_{n=0}^{\infty} b_n |n\rangle \tag{14.184}$$

where

$$b_n = \frac{e^{-\frac{N}{2}}N^{\frac{n}{2}}}{\sqrt{n!}} , \quad \frac{N}{2} = \frac{m\omega}{4\hbar}\lambda^2$$
 (14.185)

or

$$P_n = \text{ probability of finding the system in the state } |n\rangle$$
$$= |b_n|^2 = \frac{e^{-N}N^n}{n!}$$
(14.186)

which is a Poisson distribution. Thus, we obtain the coherent states once again. Let us now return to the original discussion. In the state $|\alpha\rangle$ we have

$$\hat{a} |\alpha\rangle = \alpha |\alpha\rangle \rightarrow \langle \alpha | \hat{a}^{+} = \alpha^{*} \langle \alpha |$$
 (14.187)

so that

$$\langle E \rangle = \langle \alpha | \hat{H} | \alpha \rangle = \hbar \omega \langle \alpha | (\hat{N} + 1/2) \rangle | \alpha \rangle = \hbar \omega \left(|\alpha|^2 + 1/2 \right)$$
(14.188)

$$\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle \alpha | (\hat{a} + \hat{a}^{+}) | \alpha \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\alpha + \alpha^{*})$$
(14.189)

$$\langle p \rangle = -i\sqrt{\frac{m\hbar\omega}{2}} \langle \alpha | (\hat{a} - \hat{a}^{+}) | \alpha \rangle = i\sqrt{\frac{m\hbar\omega}{2}} (\alpha^{*} - \alpha)$$
(14.190)

$$(\Delta x)^{2} = \frac{\hbar}{2m\omega} \langle \alpha | (\hat{a} + \hat{a}^{+})^{2} | \alpha \rangle - \langle x \rangle^{2}$$

$$= \frac{\hbar}{2m\omega} \left[(\alpha + \alpha^{*})^{2} + 1 \right] - \frac{\hbar}{2m\omega} (\alpha + \alpha^{*})^{2}$$

$$= \frac{\hbar}{2m\omega} \rightarrow \Delta x = \sqrt{\frac{\hbar}{2m\omega}}$$
(14.191)

$$(\Delta p)^{2} = -\frac{m\hbar\omega}{2} \langle \alpha | (\hat{a} - \hat{a}^{+})^{2} | \alpha \rangle - \langle p \rangle^{2}$$
$$= -\frac{m\hbar\omega}{2} \left[(\alpha - \alpha^{*})^{2} - 1 \right] + \frac{m\hbar\omega}{2} (\alpha^{*} - \alpha)^{2}$$
$$= \frac{m\hbar\omega}{2} \rightarrow \Delta p = \sqrt{\frac{m\hbar\omega}{2}}$$
(14.192)

Therefore, the Heisenberg inequality becomes an equality in this case

$$\Delta x \Delta p = \frac{h}{2} \tag{14.193}$$

independent of the value of α .

We can find the wave functions corresponding to $|\alpha\rangle$ using the earlier method. We have in the position representation:

$$\langle X | \hat{a} | \alpha \rangle = \alpha \langle X | \alpha \rangle = \frac{1}{\sqrt{2}} \langle X | (\hat{X} + i\hat{P}) | \alpha \rangle$$
$$= \frac{1}{\sqrt{2}} X \langle X | \alpha \rangle + \frac{i}{\sqrt{2}} \left(-i\frac{\partial}{\partial X} \right) \langle X | \alpha \rangle \qquad (14.194)$$

$$\frac{1}{\sqrt{2}} \left(X + \frac{\partial}{\partial X} \right) \langle X \mid \alpha \rangle = \alpha \langle X \mid \alpha \rangle$$
$$\rightarrow \langle X \mid \alpha \rangle = A e^{-(X - \alpha \sqrt{2})^2/2} = \psi_{\alpha}(X)$$
(14.195)

and in the momentum representation:

$$\langle P | \hat{a} | \alpha \rangle = \alpha \langle P | \alpha \rangle = \frac{1}{\sqrt{2}} \langle P | (\hat{X} + i\hat{P}) | \alpha \rangle$$
$$= \frac{1}{\sqrt{2}} i \frac{\partial}{\partial P} \langle P | \alpha \rangle + \frac{i}{\sqrt{2}} P \langle p | \alpha \rangle \qquad (14.196)$$
$$\frac{1}{\sqrt{2}} \left(P + \frac{\partial}{\partial P} \right) \langle P | \alpha \rangle = \alpha \langle P | \alpha \rangle$$

 $\rightarrow \langle P \mid \alpha \rangle = A' e^{-(P+i\alpha\sqrt{2})^2/2} = \phi_{\alpha}(P) \qquad (14.197)$

Suppose that at time t = 0, the oscillator is in a quasi-classical state $|\psi(0)\rangle = |\alpha_0\rangle$ with $\alpha_0 = \rho e^{i\varphi}$ where ρ is a real positive number. Then at a later time t

$$\begin{split} |\psi(t)\rangle &= |\alpha_0, t\rangle = e^{-\frac{1}{2}|\alpha_0|^2} \sum_{n=0}^{\infty} \frac{\alpha_0^n}{\sqrt{n!}} |n, t\rangle \\ &= e^{-\frac{1}{2}|\alpha_0|^2} \sum_{n=0}^{\infty} \frac{\alpha_0^n}{\sqrt{n!}} e^{-i\frac{E_n}{\hbar}t} |n\rangle \\ &= e^{-\frac{1}{2}|\alpha_0|^2} e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{\alpha_0^n}{\sqrt{n!}} e^{-in\omega t} |n\rangle \\ &= e^{-i\omega t/2} |\alpha(t)\rangle \end{split}$$
(14.198)

where $\alpha(t) = \alpha_0 e^{-i\omega t} = \rho e^{-i(\omega t - \varphi)}$.

Finally, we have

$$\langle \alpha, t | \hat{x} | \alpha, t \rangle = \sqrt{\frac{\hbar}{2m\omega_0}} b_0^2 \sum_k \frac{1}{k!} |\alpha|^{2k} \left(\alpha e^{-i\omega_0 t} + \alpha^* e^{i\omega_0 t} \right)$$

$$= 2\sqrt{\frac{\hbar}{2m\omega_0}} |\alpha| \cos(\omega_0 t - \phi) (b_0^2 \sum_k \frac{|\alpha|^{2k}}{k!}) \quad , \quad x_0 = \sqrt{\frac{\hbar}{2m\omega_0}}$$

$$= x_0 \cos(\omega_0 t - \phi) \quad , \quad x_0 = \rho \sqrt{\frac{2\hbar}{m\omega_0}}$$

$$(14.199)$$

and

$$\langle \alpha, t | \hat{p} | \alpha, t \rangle = -p_0 \sin(\omega_0 t - \phi) \quad , \quad p_0 = \rho \sqrt{2m\hbar\omega}$$
 (14.200)

In addition, we have (for $\rho \gg 1$)

$$\frac{\Delta x}{x_0} = \frac{1}{2\rho} << 1 \quad , \quad \frac{\Delta p}{p_0} = \frac{1}{2\rho} << 1 \tag{14.201}$$

This says that the relative uncertainties in the position and momentum of the oscillator are quite accurately defined at any time. Hence the name *quasi-classical state*.

Let us look at some numbers. We consider a pendulum of length 1 meter and of

mass 1 gram and assume that the state of this pendulum can be described by a quasi-classical state. At time t = 0 we assume that the pendulum is at $\langle x(0) \rangle = 1$ micron from its classical equilibrium position, with zero mean velocity.

An appropriate choice is $\langle x(0) \rangle = x_0$, $\langle p(0) \rangle = 0 \rightarrow \phi = 0$. We also have

$$\omega = 2\pi\nu = \sqrt{\frac{g}{\ell}} = 3.13 \, s^{-1} \to \alpha(0) = 3.9 \times 10^9 \tag{14.202}$$

The relative uncertainty in the position is

$$\frac{\Delta x}{x_0} = \frac{1}{2\rho} = \frac{1}{2\alpha(0)} = 1.3 \times 10^{-10}$$
(14.203)

We note that after 1/4 period of oscillation,

$$T = \text{period} = \frac{2\pi}{\omega} \tag{14.204}$$

$$\to \alpha (T/4) = \alpha(0)e^{i\omega T/4} = \alpha(0)e^{i\pi/2} = i\alpha(0) = -3.9i \times 10^9$$
 (14.205)

14.7.2 Construction of a Schrodinger-Cat State

Suppose that during the interval [0,T] we add to the harmonic potential, the coupling (interaction)

$$\hat{W} = \hbar g \left(\hat{a}^{+} \hat{a} \right)^{2} = \hbar g \hat{N}^{2}$$
(14.206)

We will assume that $g \gg \omega, \omega T \ll 1$. Under these conditions, we can make the approximation that, during the interval [0, T], the Hamiltonian of the system is simply \hat{W} . Assume that at time t = 0, the system is in a quasi-classical state $|\psi(0)\rangle = |\alpha\rangle$.

The eigenvectors of \hat{W} are $\{|n\rangle\}$ with $\hat{W}|n\rangle = \hbar g n^2 |n\rangle$. This implies that for $|\psi(0)\rangle = |\alpha\rangle$

$$|\psi(T)\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-ign^2 T} |n\rangle$$
 (14.207)

Some special cases will be of interest later.

$$\begin{split} |\psi(T = 2\pi/g)\rangle &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i2\pi n^2} |n\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle = |\alpha\rangle \\ |\psi(T = \pi/g)\rangle &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\pi n^2} |n\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} (-1)^n |n\rangle = |-\alpha\rangle \end{split}$$
$$\begin{split} |\psi(T = \pi/2g)\rangle &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\pi n^2/2} |n\rangle \\ &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \frac{1}{2} \left[1 - i + (1+i)(-1)^n \right] |n\rangle \\ &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \frac{1}{\sqrt{2}} \left[e^{-i\pi/4} + e^{i\pi/4}(-1)^n \right] |n\rangle \\ &= \frac{1}{\sqrt{2}} \left[e^{-i\pi/4} |\alpha\rangle + e^{i\pi/4} |-\alpha\rangle \right] \end{split}$$
(14.208)

Now, suppose that α is pure imaginary, that is, $\alpha = i\rho$. In this case, in the state $|\alpha\rangle$, the oscillator has a zero mean position and a positive velocity.

$$\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\alpha + \alpha^*) = 0$$

$$\langle p \rangle = i \sqrt{\frac{m\hbar\omega}{2}} (\alpha^* - \alpha) = \sqrt{2m\hbar\omega}\rho$$

Similarly, in the state $|-\alpha\rangle$, the oscillator also has a zero mean position, but a negative velocity.

If $|\alpha| \gg 1$, the states $|\alpha\rangle$ and $|-\alpha\rangle$ are macroscopically different. The state (14.208) is a quantum superposition of such states. It therefore constitutes a (harmless) version of Schrödinger's cat, where we represent *dead* and *alive* cats by simple vectors in Hilbert space.

14.7.3 Quantum Superposition Versus Statistical Mixture

We now consider the properties of the state (14.208) in a macroscopic situation $|\alpha| \gg 1$. We will choose $\alpha = i\rho$ pure imaginary and we set $p_0 = \sqrt{2m\hbar\omega\rho}$.

The probability distributions for position and momentum are given by

$$Pr(X) \propto \left| e^{-i\pi/4} \langle X \mid \alpha \rangle + e^{i\pi/4} \langle X \mid -\alpha \rangle \right|^{2} \\ \propto \left| e^{-i\pi/4} e^{-(X-i\rho\sqrt{2})^{2}/2} + e^{i\pi/4} e^{-(X+i\rho\sqrt{2})^{2}/2} \right|^{2} \\ \propto e^{-X^{2}} \cos^{2} \left(\sqrt{2}X\rho - \frac{\pi}{4} \right)$$
(14.209)

$$Pr(P) \propto \left| e^{-i\pi/4} \langle P \mid \alpha \rangle + e^{i\pi/4} \langle P \mid -\alpha \rangle \right|^{2}$$

$$\propto \left| e^{-i\pi/4} e^{-(P - \rho\sqrt{2})^{2}/2} + e^{i\pi/4} e^{-(P + \rho\sqrt{2})^{2}/2} \right|^{2}$$

$$\approx e^{-(P - \rho\sqrt{2})^{2}} + e^{-(P + \rho\sqrt{2})^{2}}$$
(14.210)

where in the last expression we have used the fact that, for $\rho \gg 1$, the two Gaussians centered at $\rho\sqrt{2}$ and $-\rho\sqrt{2}$ have a negligible overlap.



These probability distributions are plotted in Figure 14.10 below for $\alpha = 5i$

Figure 14.10: X Probability Distribution



Figure 14.11: P Probability Distribution

Suppose that a physicist (Alice) prepares N independent systems all in the state (14.208) and measures the momentum of each of these systems. Suppose the measuring apparatus has a resolution δp such that:

$$\sqrt{m\hbar\omega} \ll \delta p \ll p_0 \tag{14.211}$$

For $N \gg 1$, the results of these measurements is that Alice (plotting a histogram) will find two peaks, each of which contains roughly half of the events,

centered respectively at p_0 and $-p_0$ (resembling Figure 14.11).

The state (14.208) represents the quantum superposition of two states which are macroscopically different, and therefore leads to the paradoxical situations mentioned earlier.

Another physicist (Bob) claims that the measurements done by Alice have not been performed on N quantum systems in the state (14.208), but that Alice is actually dealing with a nonparadoxical *statistical mixture*, that is, half of the N systems are in the state $|\alpha\rangle$ and the other half in the state $|-\alpha\rangle$.

Assuming that this is true, the statistical mixture of Bob leads (after N momentum measurements) to the same momentum distribution as that measured by Alice: the N/2 oscillators in the state $|\alpha\rangle$ all lead to a mean momentum p_0 and the N/2 oscillators in the state $|-\alpha\rangle$ all lead to a mean momentum $-p_0$. Up to this point, there is therefore no difference and no paradoxical behavior related to the quantum superposition (14.208).

In order to settle the matter, Alice now measures the position of each of the N independent systems, all prepared in the state (14.208). Assuming that the resolution δx of the measuring apparatus is such that

$$\delta x \ll \frac{1}{|\alpha|} \sqrt{\frac{\hbar}{m\omega}} \to \delta X \ll \frac{1}{|\alpha|} = \frac{1}{\rho}$$
 (14.212)

Alice has sufficient resolution to observe the oscillations of the function

$$\cos^2\left(\sqrt{2}X\rho - \frac{\pi}{4}\right) \tag{14.213}$$

in the distribution Pr(X). The shape of the distribution for x will therefore reproduce the probability law for X as drawn in Figure 14.10 above, that is, a modulation of period

$$\left[\hbar\pi^2/(2m\alpha^2\omega)\right]^{1/2}$$
(14.214)

with a Gaussian envelope.

We continue with the assumption that Bob is dealing with a statistical mixture. If Bob performs a position measurement on the N/2 systems in the state $|\alpha\rangle$, he will find a Gaussian distribution corresponding to the probability law

$$Pr(X) \propto |\langle X \mid \alpha \rangle|^2 \propto e^{-X^2}$$
(14.215)

He will find the same distribution for N/2 systems in the state $|-\alpha\rangle$. The sum of his results will be a Gaussian distribution, which is quite different(see Figure 14.11) from the result expected by Alice.

The position measurement should, in principle, allow one to discriminate between the quantum superposition and the statistical mixture. In our earlier discussion of numbers for a pendulum we found that $\alpha = 3.9 \times 10^9$. Therefore, the resolution δx which is necessary in order to tell the difference between a set of N systems in a quantum superposition (14.208), and a statistical mixture consisting of N/2 systems in the state $|\alpha\rangle$ and N/2 systems in the state $|-\alpha\rangle$ is given by

$$\delta x \ll \frac{1}{|\alpha|} \sqrt{\frac{\hbar}{m\omega}} \approx 5 \times 10^{-26} m \tag{14.216}$$

Clearly, it is impossible to attain such a resolution in practice!

14.7.4 The Fragility of a Quantum Superposition

In a realistic physical situation, one must take into account the coupling of the oscillator with its environment, in order to estimate how long one can discriminate between the quantum superposition (14.208), that is, the *Schrodinger cat* which is *alive and dead*, and a simple statistical mixture, that is, a set of cats (systems), half of which are alive, the other half beginning dead; each cat being *either* alive *or* dead.

If the oscillator is initially in the quasi-classical state $|\alpha_0\rangle$ and if the environment is in a state $|\xi_e(0)\rangle$, the wave function of the total system is the product of the individual wave functions, and the state vector of the total system can be written as the (tensor) product of the state vectors of the two subsystems:

$$|\Phi(0)\rangle = |\alpha_0\rangle |\chi_e(0)\rangle \tag{14.217}$$

The coupling is responsible for the damping of the oscillator's amplitude.

At a later time t, the state vector of the total system becomes

$$|\Phi(t)\rangle = |\alpha_1\rangle |\chi_e(t)\rangle \tag{14.218}$$

where $\alpha_1 = \alpha(t)e^{-\gamma t}$. The number $\alpha(t)$ corresponds to the quasi-classical state one would find in the absence of damping (evaluated earlier as $\alpha(t) = \alpha_0 e^{-i\omega t}$) and γ is a real positive number.

From earlier

$$E(t) = \hbar\omega \left(|\alpha(t)|^2 + 1/2) \right) = \hbar\omega \left(|\alpha_0|^2 e^{-2\gamma t} + 1/2) \right)$$
(14.219)

The energy decreases with time. After a time much longer than $1/\gamma$, the oscillator is in its ground state. This dissipation model corresponds to a zero temperature environment. The mean energy acquired by the environment is

$$E(0) - E(t) = \hbar\omega |\alpha_0|^2 (1 - e^{-2\gamma t}) \approx 2\hbar\omega |\alpha_0|^2 \gamma t \quad , \quad 2\gamma t << 1$$
 (14.220)

For initial states of the *Schrödinger cat* type for the oscillator, the state vector of the total system, at t = 0,

$$|\Phi(0)\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\pi/4} |\alpha_0\rangle + e^{i\pi/4} |-\alpha_0\rangle \right) |\chi_e(0)\rangle$$
(14.221)

and, at a later time t,

$$|\Phi(t)\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\pi/4} |\alpha_1\rangle \left| \chi_e^{(+)}(t) \right\rangle + e^{i\pi/4} |-\alpha_1\rangle \left| \chi_e^{(-)}(t) \right\rangle \right)$$
(14.222)

still with $\alpha_1 = \alpha(t)e^{-\gamma t}$. We assume that t is chosen such that α_1 is pure imaginary, $|\alpha_1| \gg 1$, and $|\chi_e^{(+)}(t)\rangle$ and $|\chi_e^{(-)}(t)\rangle$ are two normalized states of the environment that are a priori different (but not orthogonal).

The probability distribution of the oscillator's position, measured independently of the state of the environment, is then

$$Pr(x) = \frac{1}{2} |\langle x | \alpha_1 \rangle|^2 + \frac{1}{2} |\langle x | -\alpha_1 \rangle|^2 + Real (i \langle x | \alpha_1 \rangle^* \langle x | -\alpha_1 \rangle \langle \chi_e^{(+)}(t) | \chi_e^{(-)}(t) \rangle)$$
(14.223)

Let $\eta = \left(\chi_e^{(+)}(t) \mid \chi_e^{(-)}(t)\right)$. We then have $0 \le \eta \le 1$, η real.

This says that the probability distribution of the position keeps its Gaussian envelope, but the contrast of the oscillations (cross term) is reduced by a factor η .

The probability distribution for the momentum is given by

$$Pr(p) = \frac{1}{2} |\langle p | \alpha_1 \rangle|^2 + \frac{1}{2} |\langle p | -\alpha_1 \rangle|^2 + \eta \text{Real} \left(i \langle p | -\alpha_1 \rangle^* \langle p | \alpha_1 \rangle \right)$$
(14.224)

Since the overlap of the two Gaussians $\langle p | \alpha_1 \rangle$ and $\langle p | -\alpha_1 \rangle$ is negligible for $|\alpha_1| \gg 1$, the crossed term, which is proportional to η does not contribute significantly. We recover two peaks centered at $\pm |\alpha_1| \sqrt{2m\hbar\omega}$. The distinction between a quantum superposition and a statistical mixture can be made by position measurements. The quantum superposition leads to a modulation of spatial period

$$\left[\hbar\pi^2/(2m\alpha^2\omega)\right]^{1/2}$$
(14.225)

with a Gaussian envelope, whereas only the Gaussian is observed for a statistical mixture.

In order to see this modulation, the parameter η must not be too small, say $\eta \ge 1/10$.

In a very simple model, the environment is represented by a second oscillator, of the same mass and frequency as the first one. We will assume that this second oscillator is initially in its ground state $|\xi_e(0)\rangle = |0\rangle$. If the coupling between the two oscillators is quadratic, we can take for granted that

1. the states $|\chi_e^{(\pm)}(t)\rangle$ are quasi-classical: $|\chi_e^{(\pm)}(t)\rangle = |\pm\beta\rangle$

2. and that, for short times $(\gamma t \ll 1)$: $|\beta|^2 = 2\gamma t |\alpha_0|^2$

A simple calculation then gives

$$\langle \beta \mid -\beta \rangle = e^{-|\beta|^2} \sum_{n} \frac{\beta^{*n} (-\beta)^n}{n!} = e^{-|\beta|^2} e^{-|\beta|^2} = e^{-2|\beta|^2}$$
(14.226)

From earlier considerations we must have

$$\eta = \langle \beta \mid -\beta \rangle = e^{-2|\beta|^2} \ge 1/10 \to |\beta| \le 1$$
(14.227)

For times shorter than $1/\gamma$, the energy of the first oscillator is

$$E(t) = E(0) - 2\gamma t |\alpha_0|^2 \hbar \omega$$
 (14.228)

The energy of the second oscillator is

$$E'(t) = \hbar\omega |(\beta(t)|^{2} + 1/2) = \hbar\omega/2 + 2\gamma t |\alpha_{0}|^{2} \hbar\omega$$
 (14.229)

The total energy is conserved: the energy transferred during the time t is

$$\Delta E(t) = 2\gamma t |\alpha_0|^2 \hbar \omega = \hbar \omega |(\beta(t))|^2$$
(14.230)

In order to distinguish between a quantum superposition and a statistical mixture, we must have $\Delta E \leq \hbar \omega$. In other words, if a single energy quantum $\hbar \omega$ is transferred, it becomes problematic to tell the difference.

If we return to the numerical example of the pendulum we have the following results: with $1/2\gamma = 1$ year = $3 \times 10^7 s$, the time it takes to reach $|\beta| = 1$ is $(2\gamma |\alpha_0|^2)^{-1} \approx 2 \times 10^{-12} s$

Conclusion

Even for a system as well protected from the environment as we have assumed for the pendulum, the quantum superpositions of macroscopic states are unobservable. After a very short time, all measurements one can make on a system initially prepared in such a state coincide with those made on a statistical mixture. It is therefore not possible, at present, to observe the effects related to the paradoxical character of a macroscopic quantum superposition. However, it is quite possible to observe *mesoscopic* kittens, for systems which have a limited number of degrees of freedom and are well isolated.

14.8 The Quantum Eraser

We now investigate a quantum process where the superposition of two probability amplitudes leads to an interference phenomenon. The two amplitudes will be associated with two quantum paths as in the double slit experiment. In the investigation we will show that the interference *disappears* if an intermediate measurement gives information about which path has actually been followed. Then we will show how the interference can actually *reappear* if the path information is *erased* by a quantum device.

We consider a beam of neutrons, which are particles with charge zero and spin 1/2, propagating along the *x*-axis with velocity *v*. We will treat the motion of the neutrons classically as uniform linear motion. Only the evolution of their spin states will be treated quantum mechanically.

14.8.1 Magnetic Resonance

The eigenstates of the z component of the neutron spin are denoted $|n:\pm\rangle$. A constant uniform magnetic field $\vec{B}_0 = B_0 \hat{u}_z$ is applied along the z-axis. The magnetic moment of the neutron is denoted by $\hat{\mu} = \gamma_n \hat{S}_n$ where γ_n is the gyromagnetic ratio and \hat{S}_n is the spin operator of the neutron.

The magnetic energy levels of the neutron in the presence of the field B_0 are $E_{\pm} = \mp \gamma_n \hbar B_0/2 = \pm \hbar \omega_0/2$ where $\omega_0 = -\gamma_n B_0$.

The neutrons cross a cavity of length L between times t_0 and $t_1 = t_0 + L/v$. Inside the cavity, in addition to the constant field \vec{B}_0 , a rotating field $\vec{B}_1(t)$ is applied. The field $\vec{B}_1(t)$ lies in the (x, y) plane and has a constant angular frequency ω :

$$\dot{B}_1(t) = B_1\left(\cos\omega t\hat{u}_x + \sin\omega t\hat{u}_y\right) \tag{14.231}$$

Let $|\psi_n(t)\rangle = \alpha_+ |n:+\rangle + \alpha_- |n:-\rangle$ be the neutron spin state at time t and consider a neutron entering the cavity at time t_0 .

The Hamiltonian for the system is

$$H = \hat{\mu}_n \cdot \left(\vec{B}_0 + \vec{B}_1(t)\right) = \gamma_n \hat{S}_n \cdot \left(\vec{B}_0 + \vec{B}_1(t)\right)$$
$$= \gamma_n \left(B_0 \hat{S}_z + B_1 \left(\cos \omega t \hat{S}_x + \sin \omega t \hat{S}_y\right)\right)$$
(14.232)

which gives in the $|n:\pm\rangle$ basis

$$H = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix}$$
(14.233)

Therefore, the evolution equations are

$$H |\psi_n(t)\rangle = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix} \alpha_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \alpha_- \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
$$= i\hbar \frac{d}{dt} |\psi_n(t)\rangle = i\hbar \frac{d\alpha_+}{dt} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + i\hbar \frac{d\alpha_-}{dt} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
(14.234)

$$i\hbar\frac{d\alpha_{+}}{dt} = \frac{\hbar}{2}\omega_{0}\alpha_{+} + \frac{\hbar}{2}\omega_{1}e^{-i\omega t}\alpha_{-}$$
(14.235)

$$i\hbar\frac{d\alpha_{-}}{dt} = \frac{\hbar}{2}\omega_{1}e^{i\omega t}\alpha_{+} - \frac{\hbar}{2}\omega_{0}\alpha_{-}$$
(14.236)

 \mathbf{or}

or

$$i\frac{d\alpha_+}{dt} = \frac{1}{2}\omega_0\alpha_+ + \frac{1}{2}\omega_1e^{-i\omega t}\alpha_-$$
(14.237)

$$i\frac{d\alpha_{-}}{dt} = \frac{1}{2}\omega_1 e^{i\omega t}\alpha_{+} - \frac{1}{2}\omega_0\alpha_{-}$$
(14.238)

Defining

$$\alpha_{\pm}(t) = \beta_{\pm}(t)e^{\mp i\omega(t-t_0)/2}$$
(14.239)

we get

$$i\frac{d\beta_{+}}{dt} = \frac{\omega_{0} - \omega}{2}\beta_{+} + \frac{\omega_{1}}{2}e^{-i\omega t_{0}}\beta_{-}$$
(14.240)

$$i\frac{d\beta_{-}}{dt} = \frac{\omega - \omega_{0}}{2}\beta_{-} + \frac{\omega_{1}}{2}e^{i\omega t_{0}}\beta_{+}$$
(14.241)

which has constant coefficients.

We assume that near resonance, $|\omega - \omega_0| \ll \omega_1$, and that terms proportional to $\omega - \omega_0$ may be neglected in these equations. The equations become

$$i\frac{d\beta_{+}}{dt} = \frac{\omega_{1}}{2}e^{-i\omega t_{0}}\beta_{-}$$
(14.242)

$$i\frac{d\beta_{-}}{dt} = \frac{\omega_{1}}{2}e^{i\omega t_{0}}\beta_{+} \tag{14.243}$$

whose solution is

$$\beta_{\pm}(t) = \beta_{\pm}(t_0) \cos \frac{\omega_1(t - t_0)}{2} - i\beta_{\mp}(t_0)e^{\mp i\omega t_0} \sin \frac{\omega_1(t - t_0)}{2}$$
(14.244)

Defining

$$\varphi = \frac{\omega_1(t_1 - t_0)}{2} \quad , \quad \chi = \frac{\omega(t_1 - t_0)}{2} \quad , \quad \delta = \frac{\omega(t_1 + t_0)}{2} \quad (14.245)$$

we get

$$\alpha_{+}(t_{1}) = e^{-i\chi}\beta_{+}(t_{1}) = e^{-i\chi} \left[\alpha_{+}(t_{0})\cos\varphi - i\alpha_{-}(t_{0})e^{-i\omega t_{0}}\sin\varphi \right]$$
(14.246)

$$\alpha_{-}(t_1) = e^{i\chi}\beta_{-}(t_1) = e^{i\chi} \left[\alpha_{-}(t_0)\cos\varphi - i\alpha_{+}(t_0)e^{+i\omega t_0}\sin\varphi \right]$$
(14.247)

$$\alpha_{+}(t_{1}) = \left[\alpha_{+}(t_{0})e^{-i\chi}\cos\varphi - i\alpha_{-}(t_{0})e^{-i\delta}\sin\varphi\right]$$
(14.248)

$$\alpha_{-}(t_{1}) = \left[\alpha_{-}(t_{0})e^{i\chi}\cos\varphi - i\alpha_{+}(t_{0})e^{i\delta}\sin\varphi\right]$$
(14.249)

$$\begin{pmatrix} \alpha_{+}(t_{1}) \\ \alpha_{-}(t_{1}) \end{pmatrix} = U(t_{0}, t_{1}) \begin{pmatrix} \alpha_{+}(t_{0}) \\ \alpha_{-}(t_{0}) \end{pmatrix}$$
(14.250)

where

$$U(t_0, t_1) = \begin{pmatrix} e^{-i\chi}\cos\varphi & -ie^{-i\delta}\sin\varphi \\ -ie^{i\delta}\sin\varphi & e^{i\chi}\cos\varphi \end{pmatrix}$$
(14.251)

is the time evolution matrix.

14.8.2 Ramsey Fringes

The neutrons are initially in the spin state $|n:-\rangle$. They successively cross two identical cavities of the type described above. This is called a Ramsey configuration and it is shown in Figure 14.12 below.



Figure 14.12: Ramsey Configuration

The object A is a detecting atom described later. The same oscillating field $\vec{B}_1(t)$, is applied in both cavities. The magnitude B_1 of this field is applied so as to satisfy the condition $\varphi = \pi/4$. The constant field \vec{B}_0 is applied throughout the entire experimental setup. At the end of the setup, one measures the number of outgoing neutrons which have flipped their spin and are in the final state $|n:+\rangle$. This is done for several values of ω near $\omega = \omega_0$.

The initial state condition corresponds to

$$\alpha_+(t_0) = 0$$
 , $\alpha_-(t_0) = 1$ (14.252)

At time t_1 the state is

$$\begin{pmatrix} \alpha_{+}(t_{1}) \\ \alpha_{-}(t_{1}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\chi} & -ie^{-i\delta} \\ -ie^{i\delta} & e^{i\chi} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -ie^{-i\delta} \\ e^{i\chi} \end{pmatrix}$$
(14.253)

or

$$\psi(t_1)\rangle = \frac{1}{\sqrt{2}} \left(-ie^{-i\delta} |n:+\rangle + e^{i\chi} |n:-\rangle \right)$$
(14.254)

This says that

$$\alpha_{+}(t_{1}) = -\frac{i}{\sqrt{2}}e^{-i\delta}$$
, $\alpha_{-}(t_{1}) = \frac{1}{\sqrt{2}}e^{i\chi}$ (14.255)

and the probability of finding it in the state $|n:\pm\rangle$ is

$$P_{\pm} = \frac{1}{2} \tag{14.256}$$

The same neutron enters the second cavity at time $t'_0 = t_1 + T$, with T = D/v, where D is the distance between the two cavities. Between the two cavities the spin precesses freely about \vec{B}_0 .

We then have

$$\begin{pmatrix} \alpha_{+}(t'_{0}) \\ \alpha_{-}(t'_{0}) \end{pmatrix} = \begin{pmatrix} e^{-i\tilde{\chi}} & 0 \\ 0 & e^{i\tilde{\chi}} \end{pmatrix} \begin{pmatrix} \alpha_{+}(t_{1}) \\ \alpha_{-}(t_{1}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -ie^{-i\delta}e^{-i\tilde{\chi}} \\ e^{i\chi}e^{i\tilde{\chi}} \end{pmatrix}$$
(14.257)

where

$$\tilde{\chi} = \frac{\omega_0 T}{2} \tag{14.258}$$

so that the spin state at t'_0 is

$$\begin{pmatrix} \alpha_{+}(t'_{0}) \\ \alpha_{-}(t'_{0}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -ie^{-i\delta}e^{-i\omega_{0}T/2} \\ e^{i\chi}e^{i\omega_{0}T} \end{pmatrix}$$
(14.259)

Now let t'_1 be the time when the neutron leaves the second cavity with $t'_1 - t'_0 = t_1 - t_0 = D/v$. Now $\delta' = \omega(t'_1 + t'_0)/2$ is given by

$$t'_0 = t_1 + T \quad , \quad t'_1 = 2t_1 - t_0 + T \delta' = \omega (2t_1 - t_0 + T + t_1 + T)/2 = \omega (3t_1 + 2T - t_0)/2$$

so that (for the second cavity)

$$U' = U(t'_0, t'_1) = \begin{pmatrix} e^{-i\chi'}\cos\varphi' & -ie^{-i\delta'}\sin\varphi' \\ -ie^{i\delta'}\sin\varphi' & e^{i\chi'}\cos\varphi' \end{pmatrix}$$
(14.260)

where

$$\varphi' = \varphi = \omega_1(t_1 - t_0)/2$$
, $\chi' = \chi = \omega_1(t_1 - t_0)/2$ (14.261)

so only the parameter δ changes into $\delta^{\,\prime}.$

Thus the probability amplitude for detecting the neutron in state + after the second cavity is obtained by

1. Applying U' to the vector

$$\begin{pmatrix} \alpha_{+}(t'_{0}) \\ \alpha_{-}(t'_{0}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -ie^{-i\delta}e^{-i\omega_{0}T/2} \\ e^{i\chi}e^{i\omega_{0}T} \end{pmatrix}$$
(14.262)

2. calculating the scalar product of the result with the + state.

We have

$$\alpha_{+}(t_{1}') = \frac{1}{2} \left(-ie^{-i\delta} e^{-i\chi/2} e^{-i\omega_{0}T/2} - ie^{-i\delta'} e^{i\chi/2} e^{i\omega_{0}T/2} \right)$$
(14.263)

Since

$$\delta + \chi = \omega t_1 \quad , \quad \delta' - \chi = \frac{\omega}{2} \left(3t_1 + 2T - t_0 - t_1 + t_0 \right) = \omega \left(t_1 + T \right)$$

we get

$$\alpha_{+}(t_{1}') = \frac{1}{2}e^{-i\omega(t_{1}+T)/2} \left(e^{-i(\omega_{0}-\omega)T/2} + e^{i(\omega_{0}-\omega)T/2}\right)$$
$$= e^{-i\omega(t_{1}+T)/2} \cos\frac{(\omega_{0}-\omega)T}{2}$$
(14.264)

Therefore, the probability that the neutron spin has flipped in the two-cavity system is

$$P_{+} = \left|\alpha_{+}(t_{1}')\right|^{2} = \cos^{2}\frac{(\omega_{0} - \omega)T}{2}$$
(14.265)

With the approximation $|\omega - \omega_0| \ll \omega_1$, the probability for a spin flip in a single cavity is independent of ω and equal to 1/2. In contrast, the two-cavity result exhibits strong modulation of the spin flip probability between 1 ($\omega = \omega_0$) and 0 (($\omega_0 - \omega$) $T = \pi$). This modulation results from an interference process of the two quantum paths corresponding to:

- 1. a spin flip in 1^{st} cavity and no flip in 2^{nd} cavity
- 2. no flip in 1^{st} cavity and spin flip in 2^{nd} cavity

In practice, the velocities of the neutrons have some dispersion around the mean value v. This results in a dispersion in the time T to get from one cavity to the other. A typical experimental result giving the intensity of the outgoing beam in the + state as a function of the frequency $f = \omega/2\pi$ of the rotating field B_1 is shown in Figure 14.13 below.



Figure 14.13: Experimental Results

Since $\cos^2 \varphi/2 = (1 + \cos \varphi)/2$, the averaged probability distribution is

$$\left(\cos^2 \frac{(\omega - \omega_0)T}{2}\right) = \left(\frac{1}{2} + \frac{1}{2}\cos((\omega - \omega_0)T)\right)$$
$$= \frac{1}{2} + \frac{1}{2}\int_{-\infty}^{\infty} P(T)\cos((\omega - \omega_0)T)dT \qquad (14.266)$$

For

$$P(T) = \frac{1}{\tau\sqrt{2\pi}} e^{-(T-T_0)^2/2\tau^2}$$
(14.267)

we get

$$\left(\cos^2\frac{(\omega-\omega_0)T}{2}\right) = \frac{1}{2} + \frac{1}{2}e^{-(\omega-\omega_0)^2\tau^2/2}\cos((\omega-\omega_0)T_0)$$
(14.268)

This form agrees with the observed variation with frequency in Figure 14.13 of the experimental signal. The central maximum which is located at $\omega/2\pi = 748.8 \, kHz$ corresponds to $\omega = \omega_0$. For that value a constructive interference appears whatever the neutron velocity. The lateral maxima and minima are less peaked, however, since the position of the lateral peak is velocity dependent. The first two lateral maxima correspond to $(\omega - \omega_0)T = \pm 2\pi$. Their amplitude is reduced compared to the central peak by the exponential factor.

This experiment can be compared to a Young's double slit interference experiment with polychromatic light.

Suppose that we insert between the two cavities a device which can measure the z component of the neutron spin (how this works will be discussed shortly). We

define P_{++} as the probability of detecting a neutron in the + state between the two cavities and in the + state when it leaves the second cavity. The probability P_{++} is the product of two probabilities, namely, the probability of finding the neutron in the state + when leaving the first cavity (p = 1/2) and, knowing that it is in the + state of finding it in the + state when it leaves the second cavity (p = 1/2). This gives $P_{++} = 1/4$. Similarly, $P_{-+} = 1/4$. The sum $P_{++} + P_{-+} = 1/2$ does not display any interference, since one has measured in which cavity the neutron spin has flipped. This is very similar to the electron double slit interference experiment if one measures through which slit the electron passes.

14.8.3 Detection of the Neutron Spin State

In order to measure the spin of the neutron, one lets it interact during a time τ with a spin 1/2 atom at rest. The atom's spin operator is \hat{S}_a . Let $|a:\pm z\rangle$ be the two eigenstates of the observable \hat{S}_{az} . After the interaction between the neutron and the atom, one measures the spin of the atom. Under certain conditions (which we will derive shortly) one can deduce the spin state of the neutron after the measurement.

Let $|a:\pm x\rangle$ be the eigenstates of \hat{S}_{ax} and $|a:\pm y\rangle$ those of \hat{S}_{ay} . We can then write

$$|a:\pm x\rangle = \frac{1}{\sqrt{2}} (|a:+z\rangle \pm |a:-z\rangle)$$
 (14.269)

$$|a:\pm y\rangle = \frac{1}{\sqrt{2}} \left(|a:+z\rangle \pm i \,|a:-z\rangle\right) \tag{14.270}$$

and

$$|a:\pm y\rangle = \frac{1}{2} \left((1\pm i) |a:+x\rangle + (1\mp i) |a:-x\rangle \right)$$
 (14.271)

We assume that the neutron-atom interaction does not affect the neutron's trajectory. We represent the interaction between the neutron and the atom by a very simple model. This interaction is assumed to last a finite time τ during which the neutron-atom interaction Hamiltonian has the form

$$\hat{V} = \frac{2A}{\hbar} \hat{S}_{nz} \otimes \hat{S}_{ax} \tag{14.272}$$

where A is a constant. We neglect the action of any external field, including \tilde{B}_0 during this time, i.e., we assume the atom-neutron interaction dominates for a short period of time.

The operators \hat{S}_{nz} and \hat{S}_{ax} commute since they act on two different Hilbert spaces. Therefore,

$$\left[\hat{S}_{nz}, \hat{V}\right] = 0$$
 (14.273)

The common eigenvectors of \hat{S}_{nz} and \hat{V} and the corresponding eigenvalues are

$$|n:+\rangle \otimes |a:\pm x\rangle \quad \hat{S}_{nz} = +\hbar/2 \quad V = \pm A\hbar/2 \tag{14.274}$$

$$|n:-\rangle \otimes |a:\pm x\rangle$$
 $\hat{S}_{nz} = -\hbar/2$ $V = \mp A\hbar/2$ (14.275)

The operators \hat{S}_{nz} and \hat{V} form a complete set of commuting operators as far as the spin variables are concerned.

From now on we assume that $A\tau = \pi/2$. Suppose that the initial state of the system is

$$|\psi(0)\rangle = |n:+\rangle \otimes |a:+y\rangle \tag{14.276}$$

Expanding in terms of energy eigenstates, we get

$$\psi(0)\rangle = |n:+\rangle \otimes |a:+y\rangle = \frac{1}{2} |n:+\rangle ((1+i) |a:+x\rangle + (1-i) |a:-x\rangle)$$
(14.277)

and

$$\psi(t) = \frac{1}{2} |n:+\rangle \otimes \left((1+i) |a:+x\rangle e^{-iAt/2} + (1-i) |a:-x\rangle e^{+iAt/2} \right)$$

so that

$$|\psi(\tau)\rangle = \frac{1}{2}|n:+\rangle \otimes \left((1+i)|a:+x\rangle e^{-iA\tau/2} + (1-i)|a:-x\rangle e^{+iA\tau/2}\right)$$

which for $A\tau = \pi/2$ gives

$$|\psi(\tau)\rangle = \frac{1}{2}|n:+\rangle \otimes \left((1+i)|a:+x\rangle e^{-i\pi/4} + (1-i)|a:-x\rangle e^{+i\pi/4}\right)$$

$$= \frac{1}{2}|n:+\rangle \otimes \left((1+i)|a:+x\rangle \frac{1}{\sqrt{2}}(1-i) + (1-i)|a:-x\rangle \frac{1}{\sqrt{2}}(1+i)\right)$$

$$= \frac{1}{\sqrt{2}}|n:+\rangle \otimes (|a:+x\rangle + |a:-x\rangle) = |n:+\rangle \otimes |a:+\rangle$$
(14.278)

Similarly, if $|\psi(0)\rangle = |n:-\rangle \otimes |a:-y\rangle$ then $|\psi(\tau)\rangle = |n:-\rangle \otimes |a:-\rangle$.

Physically, this means that the neutron's spin state does not change since it is an eigenstate of \hat{V} , while the atom's spin precesses around the *x*-axis with angular frequency A. At time $\tau = \pi/2A$ it lies along the *z*-axis.

We now suppose that the initial spin state is

$$|\psi(0)\rangle = (\alpha_+ |n:+\rangle + \alpha_- |n:-\rangle) \otimes |a:+y\rangle \tag{14.279}$$

After the neutron-atom interaction described above, one measures the z-component \hat{S}_{az} of the atom's spin. The state after the interaction is(using linearity)

$$|\psi(\tau)\rangle = \alpha_{+} |n:+\rangle \otimes |a:+\rangle + \alpha_{-} |n:-\rangle |a:-\rangle$$
(14.280)

The measurement of the z-component of the atoms spin gives $+\hbar/2$ with probability $|\alpha_+|^2$ and state $|n:+\rangle \otimes |a:+\rangle$ after the measurement or $-\hbar/2$ with probability $|\alpha_-|^2$ and state $|n:-\rangle \otimes |a:-\rangle$ after the measurement. In both cases, after measuring the z-component of the atom's spin, the neutron spin state is known - it is the same as that of the measured atom. It is not necessary to let the neutron interact with another measuring apparatus in order to know the value of \hat{S}_{nz} .

14.8.4 The Actual Quantum Eraser

We have seen above that if one measures the spin state of the atom between the two cavities, the interference signal disappears. We now want to show that it is possible to recover an interference if the information left by neutron on the detecting atom is *erased* by an appropriate measurement.

A neutron, initially in the spin state -, is sent into the two-cavity system. Immediately after the first cavity, there is a detecting atom of the type described above, prepared in the spin state +y. By assumption, the spin state of the atom evolves only during the time interval τ when it interacts with the neutron.

The successive states for the neutron are:

$$\begin{split} |\psi(t_1)\rangle &= |\text{after 1st cavity and before atom interaction}\rangle \\ &= \frac{1}{\sqrt{2}} \left(-ie^{-i\delta} |n:+\rangle \otimes |a:+y\rangle + e^{i\chi} |n:-\rangle \otimes |a:+y\rangle \right) \\ |\psi(t_1+\tau)\rangle &= |\text{just after atom interaction}\rangle \\ &= \frac{1}{\sqrt{2}} \left(-ie^{-i\delta} |n:+\rangle \otimes |a:+\rangle + e^{i\chi} |n:-\rangle \otimes |a:-\rangle \right) \\ |\psi(t'_0)\rangle &= |\text{entering 2nd cavity}\rangle \\ &= \frac{1}{\sqrt{2}} \left(-ie^{-i(\delta+\omega_0 T/2)} |n:+\rangle \otimes |a:+\rangle + e^{i(\chi+\omega_0 T/2)} |n:-\rangle \otimes |a:-\rangle \\ |\psi(t'_1)\rangle &= |\text{after 2nd cavity}\rangle \\ &= \frac{1}{2} \left(\begin{array}{c} -ie^{-i(\delta+\omega_0 T/2)} \left(e^{-i\chi} |n:+\rangle - ie^{-i\delta'} |n:-\rangle \right) \otimes |a:+\rangle \\ &+ e^{i(\chi+\omega_0 T/2)} \left(-ie^{-i\delta'} |n:+\rangle + e^{i\chi} |n:-\rangle \right) \otimes |a:-\rangle \end{aligned}$$

The probability of finding the neutron in the state + at time t'_1 (after the 2nd cavity) is the sum of the probabilities for finding

- 1. the neutron in state + and the atom in state +, i.e., the square modulus of the coefficient of $|n:+\rangle \otimes |a:+\rangle$, which = 1/4 in this case)
- 2. the neutron in state + and the atom in state –, which = 1/4 in this case also).

We therefore get $P_+ = 1/4 + 1/4 = 1/2$ - there is no interference since the quantum path leading in the end to a spin flip of the neutron can be determined from the state of the atom.

At time t'_1 , Bob measures the z-component of the neutron spin and Alice measures the y-component of the atom's spin. Assume that both measurements give $+\hbar/2$.

We can write

$$|\psi(t_1')\rangle = \frac{1}{2\sqrt{2}} \begin{pmatrix} -ie^{-i(\delta+\omega_0 T/2)} \left(e^{-i\chi} |n:+\rangle - ie^{-i\delta'} |n:-\rangle \right) \otimes \left(|a:+y\rangle + |a:-y\rangle \right) \\ + e^{i(\chi+\omega_0 T/2)} \left(-ie^{-i\delta'} |n:+\rangle + e^{i\chi} |n:-\rangle \right) \otimes \left(|a:+y\rangle - |a:-y\rangle \right) \end{pmatrix}$$

The probability amplitude that Bob finds $+\hbar/2$ along the z-axis while Alice finds $+\hbar/2$ along the y-axis is the coefficient of the term $|n:+\rangle \otimes |a:+y\rangle$ in the above state. Equivalently, the probability amplitude is found by projecting the state onto $|n:+\rangle \otimes |a:+y\rangle$ and squaring. We get

$$P\left(\hat{S}_{nz} = +\hbar/2, \hat{S}_{ay} = +\hbar/2\right) = \frac{1}{8} \left|-ie^{-i(\delta + \chi + \omega_0 T/2)} - ie^{i(\chi - \delta' + \omega_0 T/2)}\right|^2$$
$$= \frac{1}{2}\cos^2\frac{(\omega - \omega_0)T}{2}$$
(14.281)

which clearly exhibits a modulation reflecting an interference phenomenon. Similarly, one finds that

$$P\left(\hat{S}_{nz} = +\hbar/2, \hat{S}_{ay} = -\hbar/2\right) = \frac{1}{2}\sin^2\frac{(\omega - \omega_0)T}{2}$$
(14.282)

which is also modulated.

Let us now discuss the following three statements:

- 1. When Alice performs a measurement on the atom, Bob sees at once an interference appear in the signal he is measuring on the neutron.
- 2. Knowing the result obtained by Alice on each event, Bob can select a subsample of his own events which displays an interference phenomenon.
- 3. The experiment corresponds to an interference between two quantum paths for the neutron spin. By restoring the initial state of the atom, the measurement done by Alice erases the information concerning which quantum path is followed by the neutron spin and thus allows interference to reappear.

Statement (1) is clearly wrong. As seen earlier, if atom A is present, Bob no longer sees oscillations (in $\omega - \omega_0$) of the probability for detecting the neutron in the state +. This probability is equal to 1/2 whatever Alice does. Notice

that if the statement were correct, this would imply instantaneous transmission of information from Alice to Bob. By seeing interference reappear, Bob would know immediately that Alice is performing an experiment, even though she may be far away.

Statement (2) is correct. If Alice and Bob put together all their results, and if they select the subsample of events for which Alice finds $+\hbar/2$, then the number of events for which Bob also finds $+\hbar/2$ varies like

$$\cos^2 \frac{(\omega - \omega_0)T}{2} \tag{14.283}$$

Thus, they recover interference for this subset of events. In the complementary set where Alice found $-\hbar/2$, the number of Bob's results giving $+\hbar/2$ varies like

$$\sin^2 \frac{(\omega - \omega_0)T}{2} \tag{14.284}$$

This search for correlation between events occurring in different detectors is a common procedure in particle physics for example.

Statement (3), although less precise but more picturesque than than statement (2), is nevertheless acceptable. The

$$\cos^2 \frac{(\omega - \omega_0)T}{2} \tag{14.285}$$

signal found earlier can be interpreted as the interference of the amplitudes corresponding to two quantum paths for the neutron spin which is initially in the state –; either its spin flips in the 1^{st} cavity, or it flips in the 2^{nd} cavity. If there exists a possibility to determine which quantum path is followed by the system, interference cannot appear. It is necessary to *erase* this information, which is carried by the atom, in order to observe *some* interference. After Alice has measured the atom's spin along the y-axis, she has, in some sense *restored* the initial state of the system, and this enables Bob to see some interference. It is questionable to say that information has been erased - one may feel that, on the contrary, extra information has been acquired. Notice that the statement does not specify in which physical quantity the interference reappears. Notice also that the order of the measurements made by Alice and Bob has no importance, contrary to what this third statement seems to imply.

Chapter 15

States and Measurement

15.1 State Preparation/Determination Density Matrix Revisited

In Chapter 6 we introduced the two basic concepts needed to discuss the formal structure of quantum mechanics.

Postulate 1 defined observables as Hermitian operators and identified their eigenvalues with the possible results of any measurement of the corresponding dynamical variable.

Postulate 2 stated that every physical system has a state (or density) operator associated with it, or, alternatively, we might say that every physical system has an associated state vector.

This means that we must have some reproducible preparation procedure, which we identify with the term state, that determines a probability distribution for each dynamical variable.

This presents us with two kinds of problems:

- 1. **State Preparation** How do we actually prepare a state that is represented by a particular state operator or state vector?
- 2. State Determination For a given system, how do we determine the state operator or state vector?

15.1.1 State Preparation

Suppose that at $t = t_0$ we have a known pure state represented by a state vector $|\psi_0\rangle$. It is always possible to mathematically(theoretically) construct a time development operator $U(t_1, t_0)$ that will generate any desired pure state via

the relation $|\psi_1\rangle = U(t_1, t_0) |\psi_0\rangle$. It is not always possible, however, to realize $U(t_1, t_0)$ in practice (in the laboratory).

Example: Consider an atom in its ground state. We can prepare an excited state or a linear combination of excited states by using a pulse of electromagnetic radiation from a laser.

If we know the initial state, the mathematical mapping is one-to-one (pure state to pure state) and invertible and thus reversible.

The more fundamental problem, however, is how do we prepare a particular state from an arbitrary unknown initial state? This mapping is not invertible and, therefore, if we are able to carry it out in the laboratory, it must involve some kind of *irreversible* process.

The fundamental laws of nature, however, are reversible, as far as we know. This means that the effective irreversibility that arises must come about by a coupling of the system to some kind of apparatus or to the environment so that we have somewhere to transfer the entropy or information that is *lost* in the irreversible process.

This says that even in the microscopic world where reversibility holds, we can have, effectively, an irreversible transformation.

Now, we know that it is always possible to prepare the lowest energy state of a system simply by waiting long enough for the system to decay into its ground state. This follows because the decay of an atomic excited state by spontaneous emission is due to the atom-electromagnetic field coupling and the survival probability of an excited state, due to this interaction, decays to zero (usually exponentially with time). This means that the probability of obtaining the ground state can be made *arbitrarily close to one just by waiting long enough*.

The method assumes that the energy of the excited state is radiated away to infinity (it never returns to the system) and that the electromagnetic field is initially in its lowest energy state since otherwise we have a nonvanishing probability for the atom to absorb energy from the field and become re-excited (no longer guaranteed to be in the ground state).

In thermal equilibrium, the probability of obtaining an excited atomic state is proportional to e^{-E_x/k_BT} where $E_x =$ excitation energy of the atomic state, $k_B =$ Boltzmann constant and T = the effective temperature of the radiation field. This factor is usually very small. The presence of the cosmic background radiation at a temperature of $3^{\circ}K \rightarrow k_BT \approx 0.0002 \ eV$ gives a lower limit to the probabilities unless special shielding and refrigeration techniques are used in any experiment. This *background* increases in importance as system gets larger since E_x gets smaller.

Suppose that this *just waiting* method can be used successfully to produce the ground state for some system. It then turns out that we can then prepare a wide range of states for a spinless particle.

Suppose that we wish to prepare the state characterized by the state function

$$\psi(\vec{r}) = R(\vec{r})e^{iS(\vec{r})} \tag{15.1}$$

where $R(\vec{r})$ and $S(\vec{r})$ are real functions.

Step #1

Construct a potential $W_1(\vec{r})$ such that

$$-\frac{\hbar^2}{2m}\nabla^2\psi_0 + W_1\psi_0 = E\psi_0$$
(15.2)

where $\psi_0(\vec{r}) = R(\vec{r})$ is the ground state wave function for the system. By definition of the ground state, $R(\vec{r})$ is then a *nodeless* function. We can do this by choosing

$$W_1(\vec{r}) = E + \frac{\hbar^2}{2m} \frac{\nabla^2 R(\vec{r})}{R(\vec{r})}$$
(15.3)

Proof: Direct substitution gives

$$-\frac{\hbar^2}{2m}\nabla^2\psi_0 + W_1\psi_0 = -\frac{\hbar^2}{2m}\nabla^2\psi_0 + E\psi_0 + \frac{\hbar^2}{2m}\frac{\nabla^2 R(\vec{r})}{R(\vec{r})}\psi_0 = E\psi_0$$

or

$$\left(\nabla^2 R\right)\psi_0 - \left(\nabla^2 \psi_0\right)R = 0 \tag{15.4}$$

which certainly has a solution $\psi_0(\vec{r}) = R(\vec{r})$.

Step #2

Wait until the probability that the system has decayed to its ground state is sufficiently close to one.

Step #3

Apply a pulse potential

$$W_2(\vec{r},t) = -\hbar S(\vec{r})\delta_{\varepsilon}(t) \tag{15.5}$$

where

$$\delta_{\varepsilon}(t) = \begin{cases} 1/\varepsilon & 0 < t < \varepsilon \\ 0 & \text{otherwise} \end{cases}$$
(15.6)

During the short time interval $0 < t < \varepsilon$ we can approximate the Schrödinger equation by

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = W_2(\vec{r},t)\psi(\vec{r},t)$$
(15.7)

since W_2 overwhelms any other interactions in the limit $\varepsilon \to 0$.

Step #4

Integrate the equation with the initial condition $\psi(\vec{r}, 0) = R(\vec{r})$. We get

$$\psi(\vec{r}, 0+\varepsilon) = R(\vec{r})e^{iS(\vec{r})} \tag{15.8}$$

which is the state we wanted to prepare.

In general, we can usually carry out this procedure since we are only limited by our ability to produce the potentials W_1 and W_2 in the laboratory.

The Filtering Method

An example of this method is the Stern-Gerlach(SG) apparatus. Its mode of operation is simple. The potential energy of a magnetic moment $\vec{\mu}$ in a magnetic field \vec{B} is $E = -\vec{\mu} \cdot \vec{B}$. If the magnetic field is spatially inhomogeneous, then a force arises given by

$$\vec{F} = -\nabla E = \nabla \left(\vec{\mu} \cdot \vec{B} \right) \tag{15.9}$$

The magnitude and sign of the force depends on the spin state since $\vec{\mu} \propto \vec{S}(\text{spin})$. Therefore, different spin states will be deflected by this force into sub-beams propagating in different directions.

Thus, the SG apparatus physically separates spin states in space.

By blocking off and thus eliminating all but one of the sub-beams, which is an *irreversible* process, we can *select*(or *filter out*) a particular spin state. We will discuss this procedure in detail shortly.

No-Cloning Theorem

Why don't we just make exact replicas, or *clones*, of a prototype of the state (assuming we can find one)? We do this all the time in the world of macro-physics, i.e., duplicate keys, copying a computer file, etc.

Mathematically, to clone an arbitrary quantum state $|\varphi\rangle$ we would need a device in some suitable state $|\psi\rangle$ and a unitary time development operator \hat{U} such that

$$\hat{U}|\varphi\rangle \otimes |\psi\rangle = |\varphi\rangle \otimes |\varphi\rangle \otimes |\psi'\rangle \tag{15.10}$$

The dimension of the final device state vector $|\psi'\rangle$ is smaller than that of the initial device state vector $|\psi\rangle$ because the overall dimension of the space is

conserved under unitary transformations, i.e., if $|\varphi\rangle$ is a 1-particle state and $|\psi\rangle$ is an *N*-particle state, then $|\psi'\rangle$ must be an (N-1)-particle state.

We now show that such a device is impossible. We do it by assuming that it is possible and then arriving at a contradiction.

So, we assume it is possible to find a \hat{U} operator. Then, we assume that there exists two arbitrary states $|\varphi_1\rangle$ and $|\varphi_2\rangle$ for which the cloning transformation works, i.e.,

$$\hat{U} |\varphi_1\rangle \otimes |\psi\rangle = |\varphi_1\rangle \otimes |\varphi_1\rangle \otimes |\psi'\rangle$$

$$\hat{U} |\varphi_2\rangle \otimes |\psi\rangle = |\varphi_2\rangle \otimes |\varphi_2\rangle \otimes |\psi''\rangle$$

It is possible that the final device states $|\psi'\rangle$ and $|\psi''\rangle$ have a dependence on the state we are attempting to clone.

Now \hat{U} is a linear operator. This implies that for the superposition state

$$|\varphi_S\rangle = \frac{1}{\sqrt{2}} \left(|\varphi_1\rangle + |\varphi_2\rangle\right) \tag{15.11}$$

we must have

$$\hat{U}|\varphi_S\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}|\varphi_1\rangle \otimes |\varphi_1\rangle \otimes |\psi'\rangle + \frac{1}{\sqrt{2}}|\varphi_2\rangle \otimes |\varphi_2\rangle \otimes |\psi''\rangle$$
(15.12)

But $|\varphi_S\rangle$ is not any special state and thus, by our assumption, we should have obtained

$$\hat{U}|\varphi_S\rangle \otimes |\psi\rangle = |\varphi_S\rangle \otimes |\varphi_S\rangle \otimes |\psi'''\rangle \tag{15.13}$$

but we do not!

Thus, it is impossible to build a device to clone an arbitrary, unknown quantum state.

Classical states are just special limiting cases of quantum states. Since we are able to copy an unknown classical state, does this theorem make any sense?

We were able to prove the impossibility of cloning states because of the linearity of quantum mechanical time evolution process.

We could not prove the impossibility if we only required cloning to work on a discrete set of states. The ability in quantum mechanics to form superpositions was essential to the proof.

In any case, the set of discrete states must also be orthogonal. This follows from the fact that the inner product between state vectors is preserved by a unitary transformation. This means we must have

$$\left(\left\langle \psi \right| \otimes \left\langle \varphi_1 \right| \hat{U}^+ \right) \left(\hat{U} \left| \varphi_2 \right\rangle \otimes \left| \psi \right\rangle \right) = \left\langle \psi \right| \otimes \left\langle \varphi_1 \right| \hat{I} \left| \varphi_2 \right\rangle \otimes \left| \psi \right\rangle$$

$$= \left\langle \varphi_1 \right| \left| \varphi_2 \right\rangle \left\langle \psi \right| \psi \right\rangle$$

$$= \left(\left\langle \psi' \right| \otimes \left\langle \varphi_1 \right| \otimes \left\langle \varphi_1 \right| \right) \left(\left| \varphi_2 \right\rangle \otimes \left| \varphi'' \right\rangle \right)$$

$$= \left| \left\langle \varphi_1 \right| \left| \varphi_2 \right\rangle \right|^2 \left\langle \psi' \right| \psi'' \right\rangle$$

But since $\langle \psi | \psi \rangle = 1$, $|\langle \psi' | \psi'' \rangle| \le 1$ and $|\langle \varphi_1 | \varphi_2 \rangle| \le 1$, the relation

$$\langle \varphi_1 \mid \varphi_2 \rangle \langle \psi \mid \psi \rangle = \left| \langle \varphi_1 \mid \varphi_2 \rangle \right|^2 \langle \psi' \mid \psi'' \rangle \tag{15.14}$$

would only work mathematically if $\langle \varphi_1 | \varphi_2 \rangle = 0$ or the discrete state vectors are orthogonal.

Now, states that are classically different will certainly be orthogonal, so the no-cloning theorem that we proved for quantum states would not be in conflict with the ability to copy classical states.

Our discussion so far involves only *pure* states.

If, however, we can prepare ensembles corresponding to several different pure states $|\psi_i\rangle$, then by combining them with weights we can prepare the mixed state represented by the state operator

$$\hat{\rho} = \sum_{i} w_i |\psi_i\rangle \langle \psi_i| \tag{15.15}$$

In the laboratory, nature usually presents us with mixed states (states that are not pure) and it is the preparation of pure states that is difficult.

15.1.2 State Determination

Suppose we have some apparatus that is designed (we think) to produce a certain state. We need to be able to test or calibrate it in order to determine what state is actually being produced. In addition, some natural process can produce an unknown state and we need to be able to determine its properties.

The procedure in either case must be repeatable(whether under the control of the experimenter or occurring spontaneously in nature). This says that we must be able to create an ensemble of systems and can carry out measurements on each of them.

Because a measurement involves an interaction with the system, it will change the values of the state parameters and hence change the state representing the system. This means that any *further* measurements on the *same* system will be useless as far as enhancing our understanding of the original state. We must submit a system to the preparation procedure and then carry out only a *single* measurement on it. To obtain any more information, we must repeat the state preparation procedures before another measurement is carried out. We can use the same system each time in the preparation procedure, or another identical system each time. The results will be the same.

What sort of measurements are sufficient to determine the state operator $\hat{\rho}(\text{or state vector})$ associated with the preparation procedure?

Suppose we have a dynamical variable R whose associated operator \hat{R} has a discrete, non-degenerate eigenvalue spectrum, i.e., $\hat{R} |r_n\rangle = r_n |r_n\rangle$. Also suppose that we do a single measurement and get the result $R = r_3$. This only says that we could have any state $|\psi\rangle$ where $\langle r_3 | \psi \rangle \neq 0$ or any state operator $\hat{\rho}$ where $\langle r_3 | \hat{\rho} | r_3 \rangle \neq 0$.

If we repeat the preparation-measurement sequence many times, however, we can determine the relative frequency of the result $R = r_3$, i.e., we will be measuring

$$Prob(R = r_n | \hat{\rho}) = \langle r_n | \hat{\rho} | r_n \rangle \tag{15.16}$$

for the case of non-degenerate eigenvalues. This says that the measurement of the probability distribution of the dynamical variable R gives the *diagonal matrix elements* of the state operator in this representation.

To obtain information about the off-diagonal elements $\langle r_m | \hat{\rho} | r_n \rangle \neq 0$ we need to measure some other dynamical variable whose operator *does not* commute with R.

We can formally construct a set of operators such that their probability distributions would determine all of the matrix elements of the state operator. Consider the Hermitian operators:

$$\hat{A}_{mn} = \frac{|r_m\rangle\langle r_n| + |r_n\rangle\langle r_m|}{2} \text{ and } \hat{B}_{mn} = \frac{|r_m\rangle\langle r_n| - |r_n\rangle\langle r_m|}{2i}$$
(15.17)

We then have

$$Tr\left(\hat{\rho}\hat{A}_{mn}\right) = \sum_{p} \langle r_{p} | \hat{\rho}\hat{A}_{mn} | r_{p} \rangle$$

$$= \sum_{p} \langle r_{p} | \hat{\rho}\frac{|r_{m}\rangle\langle r_{n}| + |r_{n}\rangle\langle r_{m}|}{2} | r_{p} \rangle$$

$$= \sum_{p} \frac{1}{2} \left[\delta_{pn} \langle r_{p} | \hat{\rho} | r_{m} \rangle + \delta_{pm} \langle r_{p} | \hat{\rho} | r_{n} \rangle \right]$$

$$= \frac{1}{2} \left[\langle r_{n} | \hat{\rho} | r_{m} \rangle + \langle r_{m} | \hat{\rho} | r_{n} \rangle \right] = \operatorname{Re}\left(\langle r_{m} | \hat{\rho} | r_{n} \rangle \right)$$
(15.18)

and similarly

$$Tr\left(\hat{\rho}\hat{B}_{mn}\right) = -\mathrm{Im}\left(\langle r_m | \hat{\rho} | r_n \rangle\right) \tag{15.19}$$

Therefore, if \hat{A}_{mn} and \hat{B}_{mn} represent observables, then the measurement of their averages, i.e.,

$$Tr\left(\hat{\rho}\hat{Q}\right) = \left\langle\hat{Q}\right\rangle \tag{15.20}$$

determines the all the matrix elements of the state operator $\hat{\rho}$.

The remaining questions are

- 1. Are they observables?
- 2. How would we actually perform the necessary measurements?

These questions are not answerable within the formal approach. We must look at special cases to see what measurements are actually required.

15.1.3 Spin State (S = 1/2)

What is the most general state operator for a spin = 1/2 system? Since this is a world of 2×2 matrices and in that world the four matrices \hat{I} , $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ form a basis for all the 2×2 matrices or, equivalently, all the operators in the spin = 1/2 world. Therefore, we can always write

$$\hat{\rho} = \frac{1}{2} \left(\hat{I} + \vec{a} \cdot \hat{\sigma} \right) \tag{15.21}$$

This has $Tr(\hat{\rho}) = 1$ as required. If we choose a_x , a_y and a_z real, then $\hat{\rho} = \hat{\rho}^+$ so that it is Hermitian. We can determine a_x , a_y and a_z as follows:

$$\langle \hat{\sigma}_x \rangle = Tr\left(\hat{\rho}\hat{\sigma}_x\right) = \frac{1}{2}Tr\left(\hat{\sigma}_x + a_x\hat{\sigma}_x^2 + a_y\hat{\sigma}_y\hat{\sigma}_x + a_z\hat{\sigma}_z\hat{\sigma}_x\right)$$
$$= \frac{1}{2}Tr\left(\hat{\sigma}_x + a_x\hat{I} - ia_y\hat{\sigma}_z + ia_z\hat{\sigma}_y\right) = \frac{1}{2}a_xTr\left(\hat{I}\right) = a_x$$
(15.22)

and similarly $\langle \hat{\sigma}_y \rangle = a_y$ and $\langle \hat{\sigma}_z \rangle = a_z$ or $\langle \hat{\sigma} \rangle = Tr(\hat{\rho}\hat{\sigma}) = \vec{a}$. Physically, therefore, \vec{a} is the *polarization vector* of the state.

The eigenvalues of $\hat{\rho}$ are $(1 \pm |\vec{a}|)/2 \ge 0 \rightarrow 0 \le |\vec{a}| \le 1$. Pure states have $|\vec{a}| = 1$ (maximum polarization) and unpolarized states have $|\vec{a}| = 0$, which says that it is isotropic and the average of any spin component is zero. Thus, in order to determine the state operator, we must determine the components of \vec{a} . We have

$$\hat{S}_i = \frac{1}{2}\hbar\hat{\sigma}_i \rightarrow \left\langle \hat{S}_i \right\rangle = \frac{1}{2}\hbar Tr\left(\hat{\rho}\hat{\sigma}_i\right) = \frac{1}{2}\hbar a_i \tag{15.23}$$

and it therefore sufficient to measure

$$\langle \hat{S}_x \rangle$$
, $\langle \hat{S}_y \rangle$ and $\langle \hat{S}_z \rangle$ (15.24)

which can be done using an SG apparatus (see discussion later in this chapter).

For some unit vector $\hat{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ we have the operator

$$\hat{n} \cdot \hat{\sigma} = \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}$$
(15.25)

Its eigenvalues are given by the characteristic equation

$$-(\cos\theta - \lambda)(\cos\theta + \lambda) - \sin^2\theta = 0$$
$$\lambda^2 = 1 \rightarrow \lambda = \pm 1$$

The eigenvectors of $\hat{n} \cdot \hat{\sigma}$ are

$$\begin{bmatrix} e^{-i\varphi/2}\cos\frac{\theta}{2} \\ e^{i\varphi/2}\sin\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} -e^{-i\varphi/2}\sin\frac{\theta}{2} \\ e^{i\varphi/2}\cos\frac{\theta}{2} \end{bmatrix}$$
(15.26)

Only the relative magnitudes and relative phases of the components of any state vector have physical significance (the norm and overall phase are irrelevant). Looking at the eigenvectors, it is clear that all possible values of the relative magnitude and relative phase can be obtained by varying θ and φ , or, in other words, the relative magnitude and relative phase of any 2-component vector uniquely determines θ and φ . This implies that any pure state vector of an S = 1/2 system can always be associated with a spatial direction \hat{n} for which it is the +*hbar*/2 eigenvector for that component of spin, i.e., emphany pure state always represents a definite spin in some direction in this case.

15.1.4 Spin State (S =1)

In this case, the state operator $\hat{\rho}$ is a 3 × 3 Hermitian matrix(or operator). It depends on 8 independent real numbers (parameters), i.e., since

$$\begin{split} \hat{\rho} &= \hat{\rho}^+ \to \rho_{11}, \rho_{22}, \rho_{33} \quad real \\ &\to \rho_{ij} = \rho^*_{ii} \quad i \neq j \end{split}$$

the eight associated real numbers are

$$\rho_{11}, \rho_{22}, Re\rho_{12}, Im\rho_{12}, Re\rho_{13}, Im\rho_{13}, Re\rho_{23}, Im\rho_{23}$$

$$\rho_{33} = 1 - \rho_{11} - \rho_{22} \text{since} Tr\hat{\rho} = 1$$

We can determine three of these numbers by measuring

$$\langle \hat{S}_x \rangle, \langle \hat{S}_y \rangle, \langle \hat{S}_z \rangle$$
 (15.27)

where

$$\langle \hat{S} \rangle$$
 = polarization, as before. (15.28)

The five other parameters are obtained by measuring the average values of the so-called *quadrupole* operators

$$\hat{S}_{\alpha}\hat{S}_{\beta} + \hat{S}_{\beta}\hat{S}_{\alpha} \qquad \alpha, \beta = x, y, z \tag{15.29}$$

Only five of the six possible different operators are independent, namely,

$$(\alpha, \beta) = (x, y), (z, x), (y, z), (x, x), (y, y)$$
(15.30)

 $(\alpha, \beta) = (z, z)$ is not independent since

$$\hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = 2\hbar^2 \tag{15.31}$$

Now for spin = 1 we have the matrix representation (\hat{S}_z is diagonal)

$$\hat{S}_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0 \end{bmatrix}, \ \hat{S}_y = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0 \end{bmatrix}, \ \hat{S}_z = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1 \end{bmatrix}$$

and we have

$$\hat{n} \cdot \hat{S} = \begin{bmatrix} \cos\theta & \frac{1}{\sqrt{2}}\sin\theta e^{-i\varphi} & 0\\ \frac{1}{\sqrt{2}}\sin\theta e^{i\varphi} & 0 & \frac{1}{\sqrt{2}}\sin\theta e^{-i\varphi}\\ 0 & \frac{1}{\sqrt{2}}\sin\theta e^{i\varphi} & -\cos\theta \end{bmatrix}$$
(15.32)

with eigenvalues/eigenvectors

$$\begin{array}{ccc} & + \hbar & 0 & -h \\ \left[\begin{array}{c} \frac{1}{2}(1 + \cos\theta)e^{-i\varphi} \\ \frac{1}{\sqrt{2}}\sin\theta \\ \frac{1}{2}(1 - \cos\theta)e^{i\varphi} \end{array} \right] & \left[\begin{array}{c} \frac{1}{\sqrt{2}}\sin\theta e^{-i\varphi} \\ \cos\theta \\ \frac{1}{\sqrt{2}}\sin\theta e^{i\varphi} \end{array} \right] & \left[\begin{array}{c} \frac{1}{2}(1 - \cos\theta)e^{-i\varphi} \\ -\frac{1}{\sqrt{2}}\sin\theta \\ \frac{1}{2}(1 + \cos\theta)e^{i\varphi} \end{array} \right] \end{array}$$

Unlike the spin = 1/2 case, it is no longer true that every vector must be an eigenvector of the component of spin in some direction. This is so because it requires four real parameters to specify the relative magnitudes and the relative phases of the components of a general 3-component vector. The eigenvectors above only contain two parameters θ and φ , however. Therefore, the pure states of a spin = 1 system need not be associated with a spin eigenvalue in any spatial direction. Let us define the quantities

$$a_{\alpha} = \frac{1}{\hbar} Tr(\hat{\rho}\hat{S}_{\alpha}) \qquad \alpha = x, y, z$$

$$q_{\alpha\alpha} = \frac{1}{\hbar^2} Tr(\hat{\rho}\hat{S}_{\alpha}^2) \qquad \alpha = x, y$$

$$q_{\alpha\beta} = \frac{1}{\hbar^2} Tr[\hat{S}_{\alpha}\hat{S}_{\beta} + \hat{S}_{\beta}\hat{S}_{\alpha}] \qquad \alpha\beta = xy, yz, zx$$

these are the eight real numbers we need defined in terms of the measurable quantities:

$$\begin{array}{ll} \left\langle \hat{S}_{\alpha} \right\rangle & \alpha = x, y, z \quad , \\ \left\langle \hat{S}_{\alpha}^{2} \right\rangle & \alpha = x, y \\ \left\langle \hat{S}_{\alpha} \hat{S}_{\beta} + \hat{S}_{\beta} \hat{S}_{\alpha} \right\rangle & \alpha \beta = xy, yz, zx \end{array}$$

Now, we can do direct evaluations of the type

$$a_{x} = \frac{1}{\hbar} Tr(\hat{\rho}\hat{S}_{x})$$
$$= \frac{1}{\hbar} \sum_{s_{z}} \sum_{s'_{z}} \langle s_{z} | \hat{\rho} | s'_{z} \rangle \langle s'_{z} | \hat{S}_{x} | s_{z} \rangle$$
$$= \sqrt{2} (\rho_{12} + \rho_{23})$$

where $\left|1\right\rangle=\left|s_{z}=+\hbar\right\rangle$, $\left|2\right\rangle=\left|s_{z}=0\right\rangle$, $\left|3\right\rangle=\left|s_{z}=-\hbar\right\rangle.$

Writing down all such possible equations and solving them for the matrix elements of the state operator we can express the most general state operator as

$$\hat{\rho} = \begin{bmatrix} 1 + \frac{1}{2}(a_x - q_{xx} - q_{yy}) & \frac{1}{2\sqrt{2}}(a_x + q_{xx} - i(a_y + q_{yz})) & \frac{1}{2}(q_{xx} - q_{yy} - iq_{xy}) \\ \frac{1}{2\sqrt{2}}(a_x + q_{xx} + i(a_y + q_{yz})) & -1 + q_{xx} + q_{yy} & \frac{1}{2\sqrt{2}}(a_x - q_{xx} - i(a_y - q_{yz})) \\ \frac{1}{2}(q_{xx} - q_{yy} + iq_{xy}) & \frac{1}{2\sqrt{2}}(a_x - q_{xx} + i(a_y - q_{yz})) & 1 - \frac{1}{2}(a_x + q_{xx} + q_{yy}) \end{bmatrix}$$

With this parameterization of the state operator, we now ask how do we measure the parameters?

An SG apparatus with the magnetic field gradient along the x-direction can be used to perform measurements on an ensemble of particles that emerge from the state preparation. We can determine the relative frequencies of the S_x -values +h, 0, -h in this way. Then we can calculate

$$a_x = \frac{\langle \hat{S}_x \rangle}{\hbar} \text{ and } q_{xx} = \frac{\langle \hat{S}_x^2 \rangle}{\hbar^2}$$
 (15.33)

and similarly for gradients in the y- and z-directions. In this way we can measure $a_x, a_y, a_z, q_{xx}, q_{yy}, q_{zz}$ which provides a check since we must have $q_{zz} = 2 - q_{xx} + q_{yy}$. What about q_{xy}, q_{yz}, q_{zx} ? Here we take advantage of the time evolution of the unknown state operator $\hat{\rho}$ in a uniform magnetic field \vec{B} . We have

$$\hat{H} = -\vec{\mu} \cdot \vec{B} = \alpha \hat{S} \cdot \vec{B} = \beta \hat{S}_z \text{ for } \vec{B} = B\hat{z}$$
(15.34)

Now suppose that at t = 0 the state operator is $\hat{\rho}$ and the magnetic field is turned on for a time interval t, after which we measure \hat{S}_x^2 . By doing this many times for each of several t values, we can evaluate

$$\frac{d}{dt} \left. \left\langle \hat{S}_x^2 \right\rangle \right|_{t=0} \tag{15.35}$$

from the data. Now, for any observable

$$\left\langle \hat{R} \right\rangle_t = Tr\left(\hat{\rho}(t)\hat{R}\right)$$
 (15.36)

where

$$\frac{\partial \hat{\rho}(t)}{\partial t} = \frac{i}{\hbar} \left[\hat{\rho}(t), \hat{H} \right]$$
(15.37)

In the Schrodinger picture we then have

$$\begin{split} \frac{d}{dt} \left\langle \hat{R} \right\rangle_t &= \frac{d}{dt} \left(Tr\left(\hat{\rho}(t)\hat{R} \right) \right) = Tr\left(\frac{\partial \hat{\rho}}{\partial t} \hat{R} + \hat{\rho} \frac{\partial \hat{R}}{\partial t} \right) \\ &= Tr\left(-\frac{i}{\hbar} \left[\hat{H}, \hat{\rho} \right] \hat{R} + \hat{\rho} \frac{\partial \hat{R}}{\partial t} \right) \\ &= Tr\left(-\frac{i}{\hbar} \left(\hat{H} \hat{\rho} \hat{R} - \hat{\rho} \hat{H} \hat{R} \right) + \hat{\rho} \frac{\partial \hat{R}}{\partial t} \right) \\ &= Tr\left(-\frac{i}{\hbar} \left(\hat{\rho} \hat{R} \hat{H} - \hat{\rho} \hat{H} \hat{R} \right) + \hat{\rho} \frac{\partial \hat{R}}{\partial t} \right) \\ &= Tr\left(\frac{i}{\hbar} \hat{\rho}(t) \left[\hat{H}, \hat{R} \right] + \hat{\rho}(t) \frac{\partial \hat{R}}{\partial t} \right) \end{split}$$

From this equation of motion we then have

$$\frac{d}{dt} \left\langle \hat{S}_x^2 \right\rangle \Big|_{t=0} = \frac{i}{\hbar} Tr\left\{ \hat{\rho} \left[\hat{H}, \hat{S}_x^2 \right] \right\} = \frac{i\beta}{\hbar} Tr\left\{ \hat{\rho} \left[\hat{S}_z, \hat{S}_x^2 \right] \right\} \\ = -\beta Tr\left\{ \hat{\rho} \left[\hat{S}_x \hat{S}_y + \hat{S}_y \hat{S}_x \right] \right\} = -\beta \hbar^2 q_{xy}$$

In a similar manner we can determine q_{yz} and q_{zx} . Thus, we have managed to determine the spin = 1 state completely. This procedure can be generalized to higher spin states.

Now let us turn to the problem of determining the orbital state for a spinless particle. The orbital state of a spinless particle can be described by the coordinate representation of the state operator

$$\langle \vec{r} | \hat{\rho} | \vec{r}' \rangle \tag{15.38}$$

This is a function of two variable \vec{r} and \vec{r}' . It is called the *density matrix*. Its diagonal elements

$$\langle \vec{r} | \hat{\rho} | \vec{r} \rangle = \left| \langle \vec{r} | \psi \rangle \right|^2 \tag{15.39}$$

yield the position probability density.

To determine the density matrix for an arbitrary state we will need the probability distributions for the position and one or more dynamical variables with operators that do not commute with the position operator. In 1933, Pauli posed this question: Are the position and momentum probability densities sufficient to determine the state?

The answer turns out to be NO!. Here is a counterexample.

Consider a pure state that is an eigenfunction of the orbital angular momentum, i.e.,

$$\psi_{nlm}(\vec{r}) = f_{nl}(r)Y_m^l(\theta,\varphi) \tag{15.40}$$

Now the states $\psi_{nl,\pm m}(\vec{r})$ both have the same position and momentum distributions, but they are distinct states of the system.

A *sufficient set* of measurements to determine the orbital state of a particle *does* not seem to be known.

15.1.5 Composite Systems

Suppose that we have a *composite* system made up of *components*, i.e., a multiparticle state is a good example. Can we define states for the components separately or only for the composite system as a whole? Is the state of a composite system determined by the state of its parts?

To answer the first question, we consider a 2–component system (components labeled 1 and 2). The basis set for the vector space is the set of direct product vectors of the form

$$|a_m b_n\rangle = |a_m\rangle \otimes |b_n\rangle \tag{15.41}$$

where

 $\{|a_m\rangle\}$ = set of basis vectors for component 1 alone $\{|b_n\rangle\}$ = set of basis vectors for component 2 alone

The average of any dynamical variable R is given by

$$\langle \hat{R} \rangle = Tr\left(\hat{\rho}\hat{R}\right) = \sum_{m,n} \langle a_m b_n | \hat{\rho}\hat{R} | a_m b_n \rangle$$

$$= \sum_{m,n} \sum_{m',n'} \langle a_m b_n | \hat{\rho} | a_{m'} b_{n'} \rangle \langle a_{m'} b_{n'} | \hat{R} | a_m b_n \rangle$$

$$(15.42)$$

Now suppose that $\hat{R}^{(1)}$ is an operator representing a dynamical variable which applies exclusively to component 1, i.e.,

$$\hat{R}^{(1)} \to \hat{R}^{(1)} \otimes \hat{I}^{(2)}$$
 (15.43)

Then we have

$$\left\langle \hat{R}^{(1)} \right\rangle = \sum_{m,n} \sum_{m',n'} \left\langle a_m b_n \right| \hat{\rho} \left| a_{m'} b_{n'} \right\rangle \left\langle a_{m'} \right| \hat{R}^{(1)} \left| a_m \right\rangle \left\langle b_{n'} \right| \hat{I}^{(2)} \left| b_n \right\rangle$$

$$= \sum_{m,n} \sum_{m',n'} \left\langle a_m b_n \right| \hat{\rho} \left| a_{m'} b_{n'} \right\rangle \left\langle a_{m'} \right| \hat{R}^{(1)} \left| a_m \right\rangle \delta_{nn'}$$

$$= \sum_{m,m',n} \left\langle a_m b_n \right| \hat{\rho} \left| a_{m'} b_n \right\rangle \left\langle a_{m'} \right| \hat{R}^{(1)} \left| a_m \right\rangle$$

$$(15.44)$$

If we define the operator

$$\hat{\rho}^{(1)} = Tr^{(2)}\hat{\rho} \rightarrow \text{ operator in the space of component 1 alone}$$
(15.45)

where $Tr^{(2)}$ means the trace over the space of component 2, then we have

$$\langle a_m | \hat{\rho}^{(1)} | a_{m'} \rangle = \sum_n \langle a_m b_n | \hat{\rho} | a_{m'} b_n \rangle$$
(15.46)

and we can write

$$\left\langle \hat{R}^{(1)} \right\rangle = \sum_{m} \sum_{m'} \left\langle a_m \right| \hat{\rho}^{(1)} \left| a_{m'} \right\rangle \left\langle a_{m'} \right| \hat{R}^{(1)} \left| a_m \right\rangle = Tr\left(\hat{\rho}^{(1)} \hat{R}^{(1)} \right)$$
(15.47)

The operator $\hat{\rho}^{(1)}$ is called the *partial (or reduced) state operator* for component 1. Similar results hold for

$$\hat{R}^{(2)} \to \hat{I}^{(1)} \otimes \hat{R}^{(2)} \to \langle \hat{R}^{(2)} \rangle = Tr\left(\hat{\rho}^{(2)}\hat{R}^{(2)}\right)$$
 (15.48)

Let us now prove that $\hat{\rho}^{(1)}$ and $\hat{\rho}^{(2)}$ are in fact state operators. We must have

$$Tr^{(1)}\hat{\rho}^{(1)} = 1$$
 , $\hat{\rho}^{(1)} = \hat{\rho}^{(1)+}$, $\langle u|\hat{\rho}^{(1)}|u\rangle \ge 0$ for all $|u\rangle$ (15.49)

Now we have

$$Tr^{(1)}\hat{\rho}^{(1)} = \sum_{m} \langle a_{m} | \hat{\rho}^{(1)} | a_{m} \rangle = \sum_{m,n} \langle a_{m}b_{n} | \hat{\rho} | a_{m}b_{n} \rangle = Tr\hat{\rho} = 1$$
$$\langle a_{m} | (\hat{\rho}^{(1)} - \hat{\rho}^{(1)+}) | a_{m'} \rangle = \sum_{n} \langle a_{m}b_{n} | (\hat{\rho} - \hat{\rho}^{+}) | a_{m'}b_{n} \rangle$$
$$= \sum_{n} \langle a_{m}b_{n} | (0) | a_{m'}b_{n} \rangle = 0 \to \hat{\rho}^{(1)} = \hat{\rho}^{(1)+}$$

To prove the last condition we assume $\langle u | \hat{\rho}^{(1)} | u \rangle < 0$ and look for a contradiction. In the space of component 1 we use the orthonormal basis $\{|u_m\rangle\}$ where $|u_1\rangle = |u\rangle$ instead of using the basis $\{|a_m\rangle\}$. We also use the product states $|u_mb_n\rangle = |u_m\rangle \otimes |b_n\rangle$. Then, our assumption implies that

$$0 > \langle u_1 | \hat{\rho}^{(1)} | u_1 \rangle = \sum_n \langle u_1 b_n | \hat{\rho} | u_1 b_n \rangle$$
 (15.50)

but this is impossible since $\hat{\rho}$ is non-negative. Thus, $\hat{\rho}^{(1)}$ and $\hat{\rho}^{(2)}$ are state operators. $\hat{\rho}^{(1)}$ is sufficient to calculate the average of any dynamical variable that belongs exclusively to component 1 and similarly for $\hat{\rho}^{(2)}$.

They are *not sufficient*, in general, for determining the state of a composite system. The reason is that they provide *no information about correlations* between components 1 and 2.

If we find

$$\left\langle \hat{R}^{(1)}\hat{R}^{(2)}\right\rangle = \left\langle \hat{R}^{(1)}\right\rangle \left\langle \hat{R}^{(2)}\right\rangle \tag{15.51}$$

for all $\hat{R}^{(1)}$ and $\hat{R}^{(2)}$, then the composite state is said to be an *uncorrelated* state. In this case, we have

This is the *only case* where the total state operator is determined by the partial state operators of the components.

Pure State Factor Theorem

If $\hat{\rho}$ is a state operator and if $\hat{\rho}^{(1)} = Tr^{(2)}\hat{\rho}$ and $\hat{\rho}^{(2)} = Tr^{(1)}\hat{\rho}$ and if $\hat{\rho}^{(1)}$ describes a pure state, then

$$\hat{\rho} = \hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)}$$
 (15.53)

i.e., a pure partial state operator must be a factor of the total state operator.

Proof : We start with a representation of $\hat{\rho}$ that guarantees nonnegativeness, namely, the spectral representation in terms of eigenvectors and eigenvalues of $\hat{\rho}$

$$\hat{\rho} = \sum_{k} \rho_k \left| \varphi_k \right\rangle \left\langle \varphi_k \right| \tag{15.54}$$

This form is nonnegative as long as the eigenvalues $\rho_k > 0$. Now let us expand the eigenvectors in terms of the product vectors

$$|\varphi_k\rangle = \sum_{m,n} C_{mn}^k |a_m b_n\rangle \tag{15.55}$$

This implies

$$\hat{\rho} = \sum_{k} \rho_k \sum_{m,n} \sum_{m',n'} C_{mn}^k C_{m'n'}^{k*} |a_m b_n\rangle \langle a_{m'} b_{n'}|$$
(15.56)

so that

$$\hat{\rho}^{(1)} = Tr^{(2)}\hat{\rho} = \sum_{r} \langle b_{r} | \left(\sum_{k} \rho_{k} \sum_{m,n} \sum_{m',n'} C_{mn}^{k} C_{m'n'}^{k*} | a_{m} b_{n} \rangle \langle a_{m'} b_{n'} | \right) | b_{r} \rangle$$

$$= \sum_{r,k} \sum_{m,n} \sum_{m',n'} \rho_{k} C_{mn}^{k} C_{m'n'}^{k*} \langle b_{r} | a_{m} b_{n} \rangle \langle a_{m'} b_{n'} | b_{r} \rangle$$

$$= \sum_{r,k} \sum_{m,n} \sum_{m',n'} C_{mn}^{k} C_{m'n'}^{k*} | a_{m} \rangle \langle a_{m'} | \delta_{rn} \delta_{rn'}$$

$$= \sum_{k} \rho_{k} \sum_{m,m'} \sum_{n} C_{mn}^{k} C_{m'n}^{k*} | a_{m} \rangle \langle a_{m'} |$$
(15.57)

Now, since this is a pure state, we must have

 $\hat{\rho}^{(1)} = |\psi\rangle\langle\psi| \tag{15.58}$

Since the original basis $\{|a_m\rangle\}$ is arbitrary, we can choose $|a_1\rangle$ = $|\psi\rangle$ which implies that

$$\hat{\rho}^{(1)} = \sum_{m,m'} |a_m\rangle \langle a_{m'}| \sum_k \rho_k \sum_n C_{mn}^k C_{m'n}^{k*} = |a_1\rangle \langle a_1|$$
(15.59)

This says that

$$\sum_{k} \rho_{k} \sum_{n} C_{mn}^{k} C_{m'n}^{k*} = \sum_{n} \sum_{k} \rho_{k} C_{mn}^{k} C_{m'n}^{k*} = 0 \text{ unless } m = m' = 1$$

or that

$$\sum_{k} \rho_k \left| C_{mn}^k \right|^2 = 0 \text{ for } m \neq 1$$
 (15.60)

Therefore, for $m \neq 1$ and any k such that $\rho_k \neq 0$ we must have $C_{mn}^k = 0$ since $\rho \ge 0$. Thus

$$\hat{\rho} = \sum_{k} \rho_{k} \sum_{n} \sum_{n'} C_{1n}^{k} C_{1n'}^{k*} |a_{1}b_{n}\rangle \langle a_{1}b_{n'}|$$

= $|a_{1}\rangle \langle a_{1}| \otimes \left(\sum_{k} \rho_{k} \sum_{n} \sum_{n'} C_{1n}^{k} C_{1n'}^{k*} |b_{n}\rangle \langle b_{n'}|\right)$ (15.61)

This is the form required by the theorem. The first factor is

$$\hat{\rho}^{(1)} = |\psi\rangle \langle \psi| = |a_1\rangle \langle a_1| \tag{15.62}$$

and the second factor is identified with

$$\hat{\rho}^{(2)} = \sum_{k} \rho_k \sum_{n} \sum_{n'} C_{1n}^k C_{1n'}^{k*} |b_n\rangle \langle b_{n'}|$$
(15.63)

Summarizing, we have shown that partial states for the components of a system can be defined, but the states of the components do not suffice for determining the state of a whole composite system. The relation between the states of the components and the composite state is very complex. The theorem helps when one component is pure, which implies that $\hat{\rho}$ factors as specified.

Now a factorization of the form $\hat{\rho} = \hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)}$ implies that there is no correlations between the components 1 and 2. Therefore, a component described by a pure state *cannot* have any correlations with the rest of the system. Does this make sense?

Consider a many-particle spin system described by the state vector

i.e., all spins are up in the z-direction. This seems like a high degree of correlation. Yet, we must interpret the product form of the state vector as an absence of correlations among the particles.

We resolve this dilemma by noting that the correlation existing here is generated from the quantum mechanical probability distributions. Since $|\psi\rangle$ is an eigenvector of the z-components of the spins, there are no fluctuations in these dynamical variables and no variability (no fluctuations) implies the degree of correlation is undefined.

If, instead, we consider the components of the spin in any direction other than z, they will be subject to fluctuation and those fluctuations will indeed be correlated in the state $|\psi\rangle$.

Correlated states of multi-component systems are called *entangled states*. Many modern quantum mechanical experiments involving *quantum reality* use entangled states, as does quantum computing.

Consider the apparatus as shown in Figure 15.1 below.



Figure 15.1: Experimental Setup

The source (inside box) emits pairs of particles in variable directions, but always with opposite momentum

$$\vec{k}_b = -\vec{k}_a$$
 , $\vec{k}_{b'} = -\vec{k}_{a'}$ (15.65)

The two output ports on each side of the source box restrict each particle to two possible directions. This says that the state of the emerging pairs is

$$|\psi_{12}\rangle = \frac{1}{\sqrt{2}} \left(\left| \vec{k}_a \right\rangle \left| \vec{k}_b \right\rangle + \left| \vec{k}_{a'} \right\rangle \left| \vec{k}_{b'} \right\rangle \right) \tag{15.66}$$

The momenta of the particles are correlated in this state. This means that if particle 1 on the right has momentum $\hbar \vec{k}_a$, then particle 2 on the left must have momentum $\hbar \vec{k}_b$ and if 1 has $\hbar \vec{k}_a'$, then 2 must have $\hbar \vec{k}_b'$.

Now by inserting mirrors in the proper places we can combine the beams a and a' on the right and combine beams b and b' on the left. Looking at only one side of the apparatus, it would appear that the amplitudes from paths a and a' should produce an interference pattern (like a double slit experiment) and similarly for paths b and b' on the left.

This, in fact, would be observed experimentally if the particles were not corre-

lated and the state was of the form

$$|\psi_{12}\rangle = |\psi_1\rangle |\psi_2\rangle \tag{15.67}$$

Correlations between the particles, in fact, leads to a qualitative difference. The 2-particle configuration space wave function will have the form

$$\psi_{12}(\vec{r}_1, \vec{r}_2) \propto e^{i(\vec{k}_a \cdot \vec{r}_1 + \vec{k}_b \cdot \vec{r}_2)} + e^{i(\vec{k}_a \cdot \vec{r}_1 + \vec{k}_b \cdot \vec{r}_2)} \tag{15.68}$$

and the position probability density is

$$|\psi_{12}(\vec{r}_1, \vec{r}_2)|^2 \propto 1 + \frac{1}{2} \Big[e^{i(\vec{k}_a - \vec{k}_{a'}) \cdot \vec{r}_1} e^{-i(\vec{k}_b - \vec{k}_{b'}) \cdot \vec{r}_2} + e^{-i(\vec{k}_a - \vec{k}_{a'}) \cdot \vec{r}_1} e^{i(\vec{k}_b - \vec{k}_{b'}) \cdot \vec{r}_2} \Big] \\ \propto 1 + \cos \Big[\vec{k}_a - \vec{k}_{a'} \big) \cdot \vec{r}_1 + (\vec{k}_b - \vec{k}_{b'}) \cdot \vec{r}_2 \Big]$$
(15.69)

This form holds only in the regions where the beams overlap. The wave function is zero outside the beams.

If you ignore particles on the left and place a screen to detect particles on the right, then the detection probability for particle 1 is given by

$$\int |\psi_{12}(\vec{r}_1, \vec{r}_2)|^2 d\vec{r}_2 \tag{15.70}$$

This is featureless, i.e., no interference pattern exists in the single particle probability density.

Only in the correlations between particles can interference be observed, i.e., if we select only those particles on the right that are detected in coincidence with particles on the left in a small volume near \vec{r}_1 , then their spatial density is proportional to

$$\int |\psi_{12}(\vec{r}_1, \vec{r}_2)|^2 \delta(\vec{r}_2) d\vec{r}_2 = 1 + \cos\left[\vec{k}_a - \vec{k}_{a'}\right) \cdot \vec{r}_1 \right]$$
(15.71)

and we do see an interference pattern.

15.2 Measurement and Interpretation of States

All experiments involve state preparation followed by a measurement. Measurement and states are so closely linked in quantum mechanics that a detailed analysis of the measurement process will allow us to devise a better interpretation of the state vector.

15.2.1 Example of Spin Measurement

We now return to a discussion of the measurement of a spin component using a Stern-Gerlach(SG) apparatus.
As we discussed earlier, its mode of operation is simple. The potential energy of a magnetic moment $\vec{\mu}$ in a magnetic field \vec{B} is $E = -\vec{\mu} \cdot \vec{B}$. If the magnetic field is spatially inhomogeneous, then a force arises given by

$$\vec{F} = -\nabla E = \nabla \left(\vec{\mu} \cdot \vec{B} \right) \tag{15.72}$$

The magnitude and sign of the force depends on the spin state since $\bar{\mu} \propto \hat{S}(\text{spin})$. Therefore, different spin states (different spin components) will be deflected by this force into sub-beams propagating in different directions. The SG apparatus physically separates spin states *in space*. By blocking off and thus eliminating all but one of the sub-beams, which is an *irreversible* process, we can *select*(or *filter out*) a particular spin state. In addition, the value of the spin component can be inferred from the *location* of the sub-beam or equivalently, the deflection of the beam. A schematic of an SG apparatus is shown in Figure 15.2 below:



Figure 15.2: Stern-Gerlach Setup

The velocity of the incident beam is in the y-direction and the magnetic field is in the xz-plane, which is transverse to the beam. Some idealizations are necessary to simplify our analysis:

- 1. the magnetic field vanishes outside of the gap between the poles
- 2. only the z-component of the field is significant
- 3. within the gap, the field has a constant gradient

This means, that relative to a coordinate origin located some distance below the magnet, the components of the magnetic field can be written as

$$B_x = B_y = 0$$
, $B_z = zB'$, $B' =$ field gradient (15.73)

In this case, the magnetic force is in the z-direction and the y-component of the velocity will be constant. We can, therefore, choose a frame of reference moving uniformly in the y-direction (with the beam velocity). In this frame the incident particle is at rest and it experiences a time-dependent magnetic field that is only nonzero during the time interval T that it takes for the beam to pass through the magnet field region. The spin Hamiltonian, $\hat{H} = -\hat{\mu} \cdot \vec{B}$, can then be written as:

$$H(t) = \begin{cases} 0 & t < 0 \\ -cz\sigma_z & 0 < t < T \\ 0 & T < t \end{cases}$$
(15.74)

Now, we must have $\nabla \cdot \vec{B} = 0$ for any magnetic field. The above magnetic field does not, in fact, satisfy this relation. We would need to have, at least, that

$$B_x = -xB', \ B_z = B_0 + zB'$$
 (15.75)

If, however, $B_x \ll B_0$, which is true in practice, then any component of the magnetic moment in the xy-plane will precess rapidly about the z-axis and the force due to B_x will average to zero. Therefore, we can use our approximate Hamiltonian.

Now suppose that the state vector for the particles is given by

$$|\psi_0\rangle = a |+\rangle + b |-\rangle t \le 0 \tag{15.76}$$

where $|\mathbf{a}^2| + |b|^2 = 1$ and $|\pm\rangle = \text{spin up/down eigenvectors of } \sigma_z$.

The time evolution of this state (equation of motion) then gives for $t \ge 0$

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t} |\psi_0\rangle = ae^{-\frac{i}{\hbar}\hat{H}t} |+\rangle + be^{-\frac{i}{\hbar}\hat{H}t} |-\rangle$$
$$= ae^{iczt/\hbar} |+\rangle + be^{-iczt/\hbar} |-\rangle$$
(15.77)

so that for $t \geq T$

$$|\psi_1\rangle = |\psi(T)\rangle = ae^{iczT/\hbar} |+\rangle + be^{-iczT/\hbar} |-\rangle$$
(15.78)

This says that the effect of the interaction is to create a correlation between the spin and the momentum of the particle. The state vector above says that

if
$$\sigma_z = +1$$
 then $P_z = +Tc$
if $\sigma_z = -1$ then $P_z = -Tc$

or that the trajectory of the particle will be deflected either up or down according to whether σ_z is positive of negative. Thus, by *observing the deflection* of the particle we can *infer* the spin value.

This demonstrates that the essential feature of any measurement procedure is the establishment of a correlation between the *dynamical variable* to be measured (spin component in this case) and some *macroscopic indicator* that can be directly observed (the beam deflection in this case).

15.2.2 A General Theorem of Measurement Theory

What are the essential ingredients of a measurement?

(I) an object and (II) an apparatus together with an interaction that produces a correlation between some dynamical variable of (I) and an

appropriate indicator variable of (II)

Suppose that we want to measure the dynamical variable R (assume it has a discrete spectrum for now) that belongs to the object (I). We assume that the corresponding operator \hat{R} possesses a complete set of eigenvectors, i.e.,

$$\hat{R}\left|r\right\rangle_{I} = r\left|r\right\rangle_{I} \tag{15.79}$$

We assume that the apparatus (II) has an indicator variable A, and a corresponding operator \hat{A} that also possesses a complete set of eigenvectors, i.e.,

$$\hat{A}|\alpha,m\rangle_{II} = \alpha |\alpha,m\rangle_{II} \tag{15.80}$$

where α is the *indicator* eigenvalue and *m* labels all the other quantum numbers needed to specify a unique eigenvector of the apparatus.

We assume that the apparatus is prepared in an initial state prior to measurement given by $|0, m\rangle_{II}$, i.e., the indicator eigenvalue α is set to zero.

Now introduce some interaction between (I) and (II) that produces a unique correspondence between the value r of the dynamical variable R of (I) and the indicator α of (II). Since the interaction causes a time development of the state vectors, the time development operator \hat{U} implicitly specifies the interaction. We can study this process further via the time development operator \hat{U} without specifying any more details of the interaction.

Suppose that the initial state of (I) is an eigenstate of the \hat{R} , say $|r\rangle_I$. Then the initial state of the combined system (I) and (II) is given by

$$|r\rangle_I \otimes |0,m\rangle_{II} \tag{15.81}$$

If we require that the measurement should not change the value of the quantity being measured, then we must have

$$\dot{U}|r\rangle_{I} \otimes |0,m\rangle_{II} = |r\rangle_{I} \otimes |\alpha_{r},m'\rangle_{II}$$
(15.82)

Clearly r is unchanged by the interaction. However, the value of m might change and the value of α changes to the value that corresponds to r, i.e., the indicator variable now tells us (or allows us to infer) that the measured value is r. Since we only care about the indicator variable, we need not put any restrictions on the changes in m.

An assumption of this form is often made in the theory of measurement. It can be significantly relaxed without affecting any of the arguments.

First, there is no reason why the state of the object (I) should not change during the interaction (in practice it usually does). It is also not necessary for the state of the apparatus to remain an eigenvector corresponding to a unique value of m. We can assume a much more general result of the form

$$\hat{U}|r\rangle_{I} \otimes |0,m\rangle_{II} = \sum_{r',m'} u_{r,m}^{r',m'}|r'\rangle_{I} \otimes |\alpha_{r},m'\rangle_{II} = |\alpha_{r};(r,m)\rangle$$
(15.83)

The labels (r, m) in the last vector are not eigenvalues but just indicate the initial state from which the vector evolved.

The only restrictions here are that the final state vector is related to the initial state vector by a unitary transformation, and that the particular value of r in the initial state vector should correspond to a unique value of the indicator α_r in the final state vector. This last condition is required if the apparatus is actually to be able to carry out a measurement.

The values of α_r that correspond to different values of r should be clearly distinguishable to the observer, i.e., they should be *macroscopically distinct* values.

In the SG example the dynamical variable being measured is the spin component σ_z and the indicator variable is the momentum P_z . In this case, therefore, the indicator variable is not *physically* separate from the object of the measurement. It only needs to be *kinematically* separate. Also in this case, we look at the deflected beams and use the position coordinates of the point where the beam strikes a screen as the indicator variable.

Now consider a general initial state for object (I) of the form

$$\psi\rangle_I = \sum_r c_r \left| r \right\rangle_I \tag{15.84}$$

This is not an eigenstate of the dynamical variable R that we are measuring. It follows, however, from the linearity of the time development operator that the final state of the system will be

$$\hat{U} |\psi\rangle_{I} \otimes |0, m\rangle_{II} = \hat{U} \left(\sum_{r} c_{r} |r\rangle_{I} \right) \otimes |0, m\rangle_{II}$$
$$= \sum_{r} c_{r} |\alpha_{r}; (r, m)\rangle = \left|\psi_{m}^{f}\right\rangle$$
(15.85)

Thus, the final state vector is a *coherent superposition of macroscopically distinct indicator eigenvectors*, which is the general theorem.

Finally, the probability, in the final state, that the indicator variable A of the apparatus (II) has the value α_r is $|c_r|^2$, which is just the same as the probability in the initial state that the dynamical variable R of the object (I) had the value r. This result is required if we are to have a faithful mapping from the initial value of r to the final value α_r .

15.2.3 The Interpretation of the State Vector

We have just seen that if the initial state is not an eigenvector of the dynamical variable being measured, then the final state vector for the whole system (object of measurement + apparatus) must be a *coherent superposition* of macroscopically distinct indicator eigenvectors.

This enables us to get a better handle on how to interpret the quantum state.

Consider two standard interpretations:

(A) A pure state $|\psi\rangle$ gives a *complete* description of an individual system. A dynamical variable represented by the operator \hat{Q} has a value q in the state $|\psi\rangle$ if and only if

$$Q|\psi\rangle = q|\psi\rangle$$

(B) A pure state describes the statistical properties of an *ensemble of similarly* prepared systems.

(A) is the more common interpretation in the literature, although it is not always made explicit. It assumes that because the state vector plays such an important role in the mathematical formalism of quantum mechanics, it must have an equally important role in the interpretation. It makes a strong correspondence between the properties of the world and the properties of the state vector.

Is it consistent with the measurement theorem, however?

Because the final state vector $|\psi_m^f\rangle$ of the measurement process is not an eigenvector of the indicator variable, (A) says that the indicator cannot have a definite value, i.e., we are in a superposition of macroscopically distinct indicator states. In other words, this superposition state implies that we have a macroscopic uncertainty.

Suppose that the indicator variable is the position of a needle on a meter or a mark on chart recorder. Suppose, also, that for two adjacent values of the measured variable, r and r', the separation between the two corresponding indicator variables α_r and $\alpha_{r'}$ is several centimeters. It would obvious to any observer that the indicator position would be well defined to within a fraction of a centimeter, but that the state vector involves a superposition of terms corresponding to values of α_r that differ by many centimeters.

Thus, it seems that an interpretation of the final state as a description of an individual system cannot be reconciled with observation.

There is no such difficulty with (B) where the state vector is simply some *ab-stract quantity* that characterizes the probability distributions of the dynamical

variables of an ensemble of similarly prepared systems (each member of the ensemble consists of an object and a measuring apparatus).

The first idea for the measurement theorem came from Schrodinger in 1935 in his now famous Cat experiment. We consider a box containing a cat, a flask of poison gas, a radioactive atom, and an automatic device which releases the poison gas when the atom decays.

If the atom were isolated, then after a time equal to one half-life, its state vector would be

$$|\psi_{atom}\rangle = \frac{1}{\sqrt{2}} \left(|undecayed\rangle + |decayed\rangle \right)$$
$$= \frac{1}{\sqrt{2}} \left(|u\rangle + |d\rangle \right)$$
(15.86)

Now the atom is coupled to the cat via the apparatus. Therefore, the state of the system after one half-life is

$$|\psi_{system}\rangle = \frac{1}{\sqrt{2}} \left(|u\rangle_{atom} |alive\rangle_{cat} + |d\rangle_{atom} |dead\rangle_{cat}\right)$$
(15.87)

This is an entangled or correlated state. It is also a superposition of macroscopically distinct states (alive cat and dead cat). This is typical of any measurement process.

Schrodinger argued the plausible interpretation that an individual system's properties are smeared over a range of values contained in the state vector. The problem with this interpretation is that it implies a macroscopic smearing for classical objects such as the unfortunate cat.

The physicists that believe interpretation (A) are now forced to introduce a new *postulate*, called *reduction of the state vector* or *collapse of the state vector*.

A new process arises during a measurement so that a transition $|\psi_m^f\rangle \rightarrow |\alpha_{r_0}; (r_0, m)\rangle$ occurs.

The process is called reduction or collapse and the final state is called the reduced state. Here the new final state vector is now an eigenstate of the indicator variable A with eigenvalue α_{r_0} corresponding to the actual observed indicator position.

The big question is - what is this new mechanism?

Proposed mechanisms

1. The reduction process is caused by an unpredictable and uncontrollable disturbance of the object by the measuring apparatus. Any interaction

between the object (I) and the apparatus (II) that might act as the cause of this disturbance must already be included in the Hamiltonian that we use to construct the time development operator.

If the interaction satisfied the minimal condition that we derived earlier (15.85)

$$\hat{U} |\psi\rangle_{I} \otimes |0, m\rangle_{II} = \hat{U} \left(\sum_{r} c_{r} |r\rangle_{I} \right) \otimes |0, m\rangle_{II}$$
$$= \sum_{r} c_{r} |\alpha_{r}; (r, m)\rangle = \left|\psi_{m}^{f}\right\rangle$$
(15.88)

for it to be a measurement interaction, then it must, as above, lead to a superposition and not to a reduced state. Therefore, it is difficult to understand how the disturbance theory can make sense.

2. The observer causes the reduction process when she reads the result of the measurement from the apparatus.

This is a variation of (1) with the observer instead of the apparatus causing the disturbance. It also makes no sense. It also leads some physicists to speculation about whether quantum mechanics can be applied to the consciousness of the observer, which is an arena we do not need to enter.

3. The reduction is caused by the environment, where the environment means the rest of the universe other than (I) and (II). The phenomenon is called *decoherence*.

Here the proponents never quite make clear which part of the environment is *essential*. If we include within (II) all these *essential* parts, then it is just another disturbance model. We will have more to say about decoherence later.

4. In proving the measurement theorem, the initial state of the apparatus was assumed to be a definite pure state $|0, m\rangle_I$. But, in fact, is an abbreviation for a set of many microscopic quantum numbers, which are never determined in any experiment. It is very improbable that they will have the same values on every repetition of the state preparation. Therefore, the initial state should not be described as a pure state, but as a mixed state involving a distribution of values. Proponents of this view assumed that this would be the way to circumvent the measurement theorem.

We can defeat the last view by re-deriving the theorem using general state operators.

15.2.4 The Measurement Theorem for General States

Instead of the pure vector $|\psi_m^i\rangle = |\psi\rangle_I |0,m\rangle_I |0,m\rangle_I$ we now assume that the initial state for the system is a more general state for the system ((I) and (II))

represented by

$$\hat{\rho}^{i} = \sum_{m} w_{m} \left| \psi_{m}^{i} \right\rangle \left\langle \psi_{m}^{i} \right| \tag{15.89}$$

where the w_m are the probabilities associated with each of the microscopic states labeled by m, where m represents the quantum numbers(large number) of the apparatus other than the indicator α . The final state must be a mixture of *indicator* eigenvalues, say of the form

$$\hat{\rho}^d = \sum_r |c_r|^2 \sum_m v_m |\alpha_r; (r,m)\rangle \langle \alpha_r; (r,m)| \qquad (15.90)$$

which is diagonal with respect to α_r .

If it were not so, then we would have a coherent superposition of macroscopically distinct "indicator position" eigenvectors, which is not allowed by interpretation A. The final state is more plausible than the reduced state, which would have prescribed a unique measurement result α_{r_0} . The new conjecture is consistent with the prediction that the result of the measurement being α_r has probability $|c_r|^2$.

This conjecture is not correct, however. The actual final state of the measurement process is given by

$$\hat{\rho}^{f} = \hat{U}\hat{\rho}^{i}\hat{U}^{+} = \sum_{m} w_{m} \left|\psi_{m}^{f}\right\rangle \left\langle\psi_{m}^{f}\right|$$
(15.91)

where $\left|\psi_{m}^{f}\right\rangle = \hat{U}\left|\psi_{m}^{i}\right\rangle$. We then get

$$\hat{\rho}^{f} = \sum_{r_{1}} \sum_{r_{2}} c_{r_{1}}^{*} c_{r_{2}} \sum_{m} w_{m} \left| \alpha_{r_{1}}; (r_{1}, m) \right\rangle \left\langle \alpha_{r_{2}}; (r_{2}, m) \right|$$
(15.92)

The terms with $\alpha_{r_1} \neq \alpha_{r_2}$ correspond to a coherent superposition of macroscopically distinct indicator eigenvectors. These non-diagonal terms do not vanish and thus the state will not reduce the diagonal form above. The measurement theorem seems to be valid for these general states as well as the pure states.

It seems that in all cases where the initial state is not an eigenstate of the dynamical variable being measured, the final state will involve coherent superpositions of macroscopically distinct indicator eigenvectors. This makes interpretation (A) untenable.

Thus, if we attempt to maintain the idea that the statistical quantum theory is, in principle, able to produce a complete description of an individual physical quantum system, then we seem to always end up in a theoretical box full of implausible results. If one, however, views the quantum mechanical description as the description of an ensemble of systems, it seems possible that the theoretical difficulties will vanish.

15.2.5 Which Wave Function?

Why then do so many physicists consider an individual particle to have its own wave function?

It turns out that taking this view seldom leads to any serious errors. This is because the predictions of quantum mechanics that are derived from a wave function consist of probabilities, and the operational significance of a probability corresponds to a relative frequency. This means that one usually has to invoke an ensemble of similar systems when one makes a comparison with experiment independent of how one interprets the wave function.

Since so many results do not seem to depend in any critical manner on which interpretation one makes, should we dismiss the subject of interpretation as irrelevant?

I do not think so!

Let us consider this interesting case. Electrons are emitted from a hot cathode and then accelerated to form a beam to be used in interference experiments.

Using interpretation (A) we can account for the energy spread in the beam via two different assumptions:

- 1. Each electron is emitted in an energy eigenstate (a plane wave), but the particular energy varies from one electron to the next.
- 2. Each electron is emitted as a wave packet which has an energy spread equal to the energy spread of the beam.

Do these two assumptions lead to quantitatively different predictions about the resulting interference and thus allow us to distinguish between them experimentally?

Let us analyze this system such that the electron beam is moving along the xaxis (a one dimensional problem). Then, assumption (1) says that each electron has a wave function of the form

$$\psi_k(x,t) = e^{i(kx - \omega t)} \tag{15.93}$$

and has an energy

$$E = \hbar\omega = \frac{\hbar^2 k^2}{2M} \tag{15.94}$$

The observed energy distribution (spread) of the beam enables us to calculate the probability density (we call it $W(\omega)$). The state operator corresponding to this process will then be

$$\hat{\rho} = \int |\psi_k\rangle \langle \psi_k | W(\omega) d\omega \qquad (15.95)$$

In the coordinate representation we get

$$\rho(x,x') \equiv \langle x | \hat{\rho} | x' \rangle = \int \psi_k(x,t) \psi_k^*(x',t) W(\omega) d\omega$$
$$= \int e^{ik(x-x')} W(\omega) d\omega \qquad (15.96)$$

Note that all of the time dependence cancels out, so that we have a steady state!

All observable quantities, including the interference pattern, can be calculated from the state function $\rho(x, x')$.

Now, assumption (2) says that if an individual electron is emitted at t_0 in a wave packet state

$$\psi_{t_0}(x,t) = \int A(\omega) e^{i(kx - \omega(t - t_0))} d\omega$$
(15.97)

then the energy distribution is given by $|A(\omega)|^2 = W(\omega)$. The state function for the emission process is obtained by averaging over the emission time (assumed to be uniformly distributed):

Now, integrating over t_0 and then taking the limit, the integral is zero unless $\omega = \omega' (k = k')$. We thus get

$$\rho(x,x') = \int |A(\omega)|^2 e^{ik(x-x')} d\omega \qquad (15.98)$$

This is the same result as obtained from assumption (1). Assumptions (1) and (2) do not lead to any observable differences and any controversy over the supposed wave functions of individual electrons seems to be pointless.

Now let us adopt interpretation (B), which was that

A pure state describes the statistical properties

of an ensemble of similarly prepared systems

We now regard the state operator $\hat{\rho}$ as the fundamental description of the state generated by the thermal emission process, which now yields an ensemble of systems each of which is a single electron. In this case, we can obtain $\rho(x, x')$ without ever speculating about individual wave functions. Since this is a steady state process we must have

$$\frac{d\hat{\rho}}{dt} = 0 \tag{15.99}$$

(in the Schrodinger picture). This implies that

$$\left[\hat{H},\hat{\rho}\right] = 0 \tag{15.100}$$

and thus \hat{H} and $\hat{\rho}$ possess a complete set of *common* eigenvectors. This set is the free particle states $|\psi_{\omega}\rangle$, which have the coordinate representation $\langle x | \psi_{\omega} \rangle = e^{ikx}$ and satisfy the eigenvalue equation $\hat{H} |\psi_{\omega}\rangle = \hbar \omega |\psi_{\omega}\rangle$. In this case the state operator has the form

$$\hat{\rho} = \int |\psi_{\omega}\rangle \langle \psi_{\omega}|W(\omega)d\omega \qquad (15.101)$$

 $W(\omega)$ again describes the energy distribution in the beam. In the coordinate representation this becomes

$$\rho(x,x') = \int e^{ik(x-x')} W(\omega) d\omega \qquad (15.102)$$

Of course we get the same result as earlier, since all of these clever approaches must agree with the same set of experimental predictions in the end!!

This last approach seems, however, to be superior since it avoids any (*probably pointless*) speculations about the form of the supposed wave function of an individual electron.

15.2.6 Spin Recombination Experiment

Is there any evidence that the state vector retains its form and does not undergo any *reduction* process?

Let us consider a spin recombination experiment involving a *single crystal neutron interferometer*. The crystal is cut into the shape shown inn Figure 15.3 below from a perfect (no dislocations or grain boundaries) crystal of silicon about 10 cm long.



Figure 15.3: Single Crystal Neutron Interferometer

The diffraction beams are shown in Figure 15.4 below: The incident beam at A is divided into a transmitted beam AC and a diffracted



Figure 15.4: Diffraction Beams

(Bragg-reflected) beam AB. Similar divisions occur at B and C, with the transmitted beams leaving the apparatus (no further role in the experiment). The diffracted beams from B and C recombine coherently at D, where a further Bragg reflection takes place. The interference of the amplitudes of the two beams is observable by means of two detectors, D_1 and D_2 .

The amplitude at D_1 is the sum of the transmitted part of CD plus the diffracted part of BD, and similarly, the amplitude at D_2 is the sum of the transmitted part of BD plus the diffracted part of CD.

We assume for simplicity that the transmission and reflection coefficients are the same at each of the vertices A, B, C and D and that free propagation of the plane waves takes place between these vertices.

Only two distinct propagation directions are involved in this experiment. At each diffraction vertex the amplitudes are redistributed between these two modes. Figure 15.5 below shows what happens at a general diffraction vertex.



Figure 15.5: Diffraction Vertex

The time evolution and propagation processes are generated by linear operators. This implies that the relation between the amplitudes of the outgoing and incoming waves is of the form

$$\begin{bmatrix} a_1' \\ a_2' \end{bmatrix} = U \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \text{ where } U = \begin{bmatrix} t & r \\ s & u \end{bmatrix}$$
(15.103)

$$a_1' = ta_1 + ra_2$$
$$a_2' = sa_1 + ua_2$$

U is a unitary matrix. The elements t an u are transmission coefficients and the elements r and s are reflection coefficients.

Because U is unitary we have these relations:

$$UU^{+} = I \to |t|^{2} + |u|^{2} = 1 \text{ and } |r|^{2} + |s|^{2} = 1$$
 (15.104)

$$\det U = 1 \rightarrow |tu - rs| = 1 \tag{15.105}$$

$$U^{-1} = U^{+} \rightarrow \frac{1}{tu - rs} \begin{bmatrix} u & -r \\ -s & t \end{bmatrix}$$
$$= \begin{bmatrix} t^{*} & s^{*} \\ r^{*} & u^{*} \end{bmatrix} \rightarrow |u| = |t| \text{ and } |s| = |r|$$
(15.106)

Now complex numbers can be regarded as 2-dimensional vectors, to which the triangle inequality

$$|a+b| \le |a|+|b| \tag{15.107}$$

applies. Using the inequality we have

$$|tu - rs| = 1 \to |tu| + |rs| \ge 1 \tag{15.108}$$

Now since |u| = |t| and |s| = |r| we must have |tu| + |rs| = 1. This result is compatible with |tu - rs| = 1 only if tu and -rs have the same complex phase, and thus rs/tu must be real and negative.

If the amplitude at A is ψ_A , then the amplitudes at B and C will be

$$\psi_B = \psi_A r e^{i\varphi_{AB}}$$
 and $\psi_C = \psi_A t e^{i\varphi_{AC}}$ (15.109)

where φ_{AB} is the phase change due to the propagation through the empty space between A and B, and similarly for φ_{AC} . The amplitude that emerges toward the detector D_1 is the sum of the amplitudes from paths $ABDD_1$ and $ACDD_1$ (and similarly for detector D_2):

$$\begin{split} \psi_{D_{1}} &= \psi_{A} \left((a'_{2}, a_{1}) e^{i\varphi_{AB}} (a'_{1}, a_{2}) e^{i\varphi_{BD}} (a'_{2}, a_{1}) + (a'_{1}, a_{1}) e^{i\varphi_{AC}} (a'_{2}, a_{1}) e^{i\varphi_{CD}} (a'_{2}, a_{2}) \right) \\ &= \psi_{A} \left(s e^{i\varphi_{AB}} e^{i\varphi_{BD}} s + t e^{i\varphi_{AC}} s e^{i\varphi_{CD}} u \right) \\ &= \psi_{A} s \left(r s e^{i\varphi_{AB}} e^{i\varphi_{BD}} + t u e^{i\varphi_{AC}} e^{i\varphi_{CD}} \right) \\ \psi_{D_{2}} &= \psi_{A} \left((a'_{2}, a_{1}) e^{i\varphi_{AB}} (a'_{1}, a_{2}) e^{i\varphi_{BD}} (a'_{1}, a_{1}) + (a'_{1}, a_{1}) e^{i\varphi_{AC}} (a'_{2}, a_{1}) e^{i\varphi_{CD}} (a'_{1}, a_{2}) \right) \\ &= \psi_{A} \left(s e^{i\varphi_{AB}} e^{i\varphi_{BD}} t + t e^{i\varphi_{AC}} s e^{i\varphi_{CD}} r \right) \\ &= \psi_{A} trs \left(e^{i\varphi_{AB}} e^{i\varphi_{BD}} + e^{i\varphi_{AC}} e^{i\varphi_{CD}} \right) \end{aligned}$$
(15.111)

or

Any perturbation that has an unequal effect on the phases associated with the two paths will influence the intensities of the beams reaching the detectors D_1 and D_2 . Since rs/tu is negative, it follows that if the interference between the two terms in ψ_{D_1} is constructive, then the interference between the two terms in ψ_{D_1} will be destructive and vice versa. The best way to detect such a perturbation is to monitor the difference between the counting rates in D_1 and D_2 .

An experiment of this sort in 1975 detected a quantum interference due to gravity. The interferometer was rotated about a horizontal axis parallel to the incident beam causing a difference in the gravitational potential on paths AC and AB and thus a phase shift in the interference pattern. In the spin recombination experiment, a beams of neutrons with spin polarized in the +z-direction is incident from the left as shown in Figure 15.6 below:



Figure 15.6: Spin Recombination Experiment

At point A the beam is split into a transmitted beam AC and a Bragg-reflected beam AB of equal intensity. Similar splitting occur at B and at C. The transmitted beams at B and C exit the apparatus. We now insert a spin-flipper into the beam CD as shown. The *dots* indicate spin up beams and the x indicates a spin down beam. The spin up and spin down beams are then recombined at D. The detectors then determine the spin state of the beams that emerge from the apparatus after point D.

We let the vectors $|+\rangle$ and $|-\rangle$ denote the spin-up and spin-down eigenvectors of $\hat{\sigma}_z$. The neutrons at point *B* have the spin state $|+\rangle$ and the neutrons after the spin-flipper have the spin state $|-\rangle$. We then ask this question.

What will be the spin state when the beams recombine at D?

At one time, when the beams are at B and C, they are separated by several centimeters. This means that their spatial wave functions do not overlap. One might suppose, in this case, that all coherence is lost and that no interference is possible, i.e., that the spin state should be an incoherent mixture of spin-up and spin-down states of the form

$$\hat{\rho}^{inc} = \frac{1}{2} \left(|+\rangle \left(+ |+|-\rangle \left(- | \right) \right)$$
(15.112)

This state would also result if we applied the reduction hypothesis.

If, on the other hand, the coherence is maintained somehow, then the spin state will be of the form

$$\hat{\rho}^{coh} = |u\rangle \langle u| \text{ where } |u\rangle = \frac{1}{\sqrt{2}} \left(e^{i\alpha} |+\rangle + e^{i\beta} |-\rangle \right)$$
(15.113)

Both of these state operators predict that $\langle \hat{\sigma}_z \rangle = 0$, i.e.

$$\begin{aligned} \left\langle \hat{\sigma}_{z} \right\rangle^{inc} &= Tr\left(\hat{\rho}^{inc}\hat{\sigma}_{z}\right) = \left\langle + | \hat{\rho}^{inc}\hat{\sigma}_{z} |+ \right\rangle + \left\langle - | \hat{\rho}^{inc}\hat{\sigma}_{z} |- \right\rangle \\ &= \left\langle + | \hat{\rho}^{inc} |+ \right\rangle - \left\langle - | \hat{\rho}^{inc} |- \right\rangle \\ &= \left\langle + | \left(\frac{1}{2}\left(|+ \rangle \left\langle + | + |- \rangle \left\langle - | \right\rangle\right)\right) |+ \right\rangle - \left\langle - | \left(\frac{1}{2}\left(|+ \rangle \left\langle + | + |- \rangle \left\langle - | \right\rangle\right)\right) |- \right\rangle \\ &= \frac{1}{2} - \frac{1}{2} = 0 \\ \left\langle \hat{\sigma}_{z} \right\rangle^{coh} &= Tr\left(\hat{\rho}^{coh}\hat{\sigma}_{z}\right) = \left\langle + | \hat{\rho}^{coh}\hat{\sigma}_{z} |+ \right\rangle + \left\langle - | \hat{\rho}^{coh}\hat{\sigma}_{z} |- \right\rangle \\ &= \left\langle + | \hat{\rho}^{coh} |+ \right\rangle - \left\langle - | \hat{\rho}^{coh} |- \right\rangle \\ &= \left\langle + | \left(|u \rangle \left\langle u |\right) |+ \right\rangle - \left\langle - | \left(|u \rangle \left\langle u |\right) |- \right\rangle = \frac{1}{2} - \frac{1}{2} = 0 \end{aligned}$$

or that the z-component of spin is equally likely to be positive or negative.

However, $\hat{\rho}^{inc}$ actually predicts zero polarization in any direction, while $\hat{\rho}^{coh}$ predicts that the spin is polarized in some direction in the xy-plane. We can see this by computing

$$\langle \hat{\sigma}_x \rangle^{coh} = Tr\left(\hat{\rho}^{coh}\hat{\sigma}_x\right) = \langle +|\hat{\rho}^{coh}\hat{\sigma}_x|+\rangle + \langle -|\hat{\rho}^{coh}\hat{\sigma}_x|-\rangle$$

$$= \langle +|\hat{\rho}^{coh}|-\rangle - \langle -|\hat{\rho}^{coh}|+\rangle = \langle +|\left(|u\rangle\langle u|\right)|-\rangle - \langle -|\left(|u\rangle\langle u|\right)|+\rangle$$

$$= \frac{1}{2} \langle +|\left(e^{i\alpha}|+\rangle + e^{i\beta}|-\rangle\right) \left(e^{-i\alpha}\langle +|+e^{-i\beta}\langle -|\right)|-\rangle$$

$$- \frac{1}{2} \langle -|\left(e^{i\alpha}|+\rangle + e^{i\beta}|-\rangle\right) \left(e^{-i\alpha}\langle +|+e^{-i\beta}\langle -|\right)|+\rangle$$

$$= \frac{1}{2} e^{i\alpha} e^{-i\beta} - \frac{1}{2} e^{-i\alpha} e^{i\beta} = \cos(\alpha - \beta)$$

$$(15.114)$$

Even though the phases α and β are not necessarily known in advance, their difference can be systematically varied by placing known phase-shifters in one of the beams. Such an experiment was done in 1982 and it found a periodic dependence of $\langle \hat{\sigma}_x \rangle$ on the phase shift and no such dependence for $\langle \hat{\sigma}_z \rangle$. This confirms that the *coherent superposition is the correct state*.

Let us look at the state operators in more detail.

If we account for both the position and spin variables, the state function(vector) should be

$$|\psi\rangle = \psi_{+}(\vec{r})|+\rangle + \psi_{-}(\vec{r})|-\rangle \qquad (15.115)$$

where the wave functions $\psi_+(\vec{r})$ and $\psi_-(\vec{r})$ vanish outside the beams. The spin state operator is given by

$$\hat{\rho} = |\psi\rangle\langle\psi| = |\psi_{+}|^{2}|+\rangle\langle+|+\psi_{+}\psi_{-}^{*}|+\rangle\langle-|+\psi_{-}\psi_{+}^{*}|-\rangle\langle+|+|\psi_{-}|^{2}|-\rangle\langle-| \qquad (15.116)$$

or

$$\rho = \begin{bmatrix} \langle +|\hat{\rho}|+\rangle & \langle +|\hat{\rho}|-\rangle \\ \langle -|\hat{\rho}|+\rangle & \langle -|\hat{\rho}|-\rangle \end{bmatrix} = \begin{bmatrix} |\psi_{+}|^{2} & \psi_{+}\psi_{-}^{*} \\ \psi_{-}\psi_{+}^{*} & |\psi_{-}|^{2} \end{bmatrix}$$
(15.117)

Along AB, AC, and from B to the left of D, $\psi_{-}(\vec{r}) = 0$ and from the right of the spin-flipper to the left of D, $\psi_{+}(\vec{r}) = 0$. Both components are nonzero to the right of D.

At the point D the off-diagonal terms are nonzero, which means that we have a coherent superposition. In this experiment, the preservation of the coherence over a distance of several centimeters is possible because the scatterer is cut from a single crystal of silicon and the relative separation of the components are stable to within the interatomic separation distance.

Suppose that the spectrometer were not such a high precision device and that the relative separations of points A, B, C, and D are subject to random fluctuations that are larger than the spatial spread of the neutron wave function.

This gives rise to random fluctuations in the phases α and β and hence, in the phases of the off-diagonal terms. Different neutrons passing through the spectrometer at different times would experience different configurations of the spectrometer, and to determine the observed statistical distributions we must average over these fluctuations.

If we regard the noise fluctuations as a part of the state preparation procedure, then ρ should be averaged over the noise. If the phase difference $(\alpha - \beta)$ fluctuates by more than 2π , then the off-diagonal terms will average to zero, ρ will be diagonal and will reduce to ρ^{inc} which corresponds to the state operator for the *reduced* state.

The *reduced* state can therefore be significant under certain conditions. It does not seem, however, to be a fundamental object, but , instead, arises only due to an effect on the system (neutron + spectrometer) from its environment(the cause of the noise fluctuations). The separation of the system and the environment is, however, artificial. If the reduction takes place in this manner, then it is not a new fundamental process, and it would not have anything to do with measurement.

Let us now include the environment not as an external effect on the system, but as an integral part of the system. The neutrons that follow path ABDwill interact differently with the environment than those that follow path ACD. These interactions will affect the state of the environment and therefore the final state must now be

$$|\psi\rangle = \psi_{+}(\vec{r})|+\rangle |e_{1}\rangle + \psi_{-}(\vec{r})|-\rangle |e_{2}\rangle$$
(15.118)

where $|e_1\rangle$ is the state of the environment if the neutron followed path ABDand $|e_2\rangle$ is the state of the environment if the neutron followed path ACD. If $|e_1\rangle = |e_2\rangle$, then this inclusion of the environment has no effect. If we recalculate the state operator we now get

$$\rho = \begin{bmatrix} |\psi_{+}|^{2} & \psi_{+}\psi_{-}^{*} \langle e_{2} | e_{1} \rangle \\ \psi_{-}\psi_{+}^{*} \langle e_{1} | e_{2} \rangle & |\psi_{-}|^{2} \end{bmatrix}$$
(15.119)

If the difference between the effects of taking paths ABD and ACD on the environment is so great that $|e_1\rangle$ and $|e_2\rangle$ are orthogonal, then the state operator reduced once again to ρ^{inc} .

We have thus seen two possible methods of handling the influences, if any, of the environment on the experiment. One method treats the effect of the environment as an outside perturbation, which introduces random phases and we lose coherence if the random phase fluctuations are large enough. In the second method, the environment is included in the state vector of the system. It is then the effect of the apparatus on the environment, rather than the environment on the apparatus, that is important. Clearly, these two approaches are equivalent.

15.2.7 Joint and Conditional Probabilities

In all of our discussions, an experiment consists of a state preparation followed by the measurement of a single quantity. Suppose, instead, of a single measurement, it involves a sequence of measurements of two or more dynamical variables. In this case, we will not only need the probability distributions for the individual quantities to be measured, but also will need to consider correlations between values of the quantities to be measured.

We can deal with this by computing the joint probability distribution for the results of two or more measurements, or the probability for one measurement conditional on both state preparation and the result of another measurement.

We discussed these joint and conditional probabilities earlier in Chapter 5. Axiom 4 related them by

$$\operatorname{Prob}(A \wedge B|C) = \operatorname{Prob}(A|C)\operatorname{Prob}(B|A \wedge C) \tag{15.120}$$

We let event C be the state preparation that corresponds to the state operator $\hat{\rho}$ so we will replace C with $\hat{\rho}$. The events A and B will be the results of two measurements following that state preparation. Let R and S be two dynamical variables represented by the Hermitian operators \hat{R} and \hat{S} such that

$$\hat{R}|r_n\rangle = r_n|r_n\rangle \text{ and } \hat{S}|s_m\rangle = s_m|s_m\rangle$$
 (15.121)

We now define two projection operators.

Let Δ be some interval (in eigenvalue space). Then the operators

$$M_R(\Delta) = \sum_{r_n \in \Delta} |r_n\rangle \langle r_n| \quad , \quad M_S(\Delta) = \sum_{s_m \in \Delta} |s_m\rangle \langle s_m| \tag{15.122}$$

project onto the subspace spanned by those eigenvectors whose eigenvalues lie in the interval Δ .

Let A denote the event of R taking a value in the range $\Delta_a(R \in \Delta_a)$. Let B denote the event of S taking a value in the range $\Delta_b(S \in \Delta_b)$.

We suppose that the first of these events takes place at time t_a and the second at time t_b . We use the Heisenberg representation and assume that the specification of t_a is implicit in the operators \hat{R} and $M_R(\Delta)$ and that the specification of t_b is implicit in the operators \hat{S} and $M_S(\Delta)$.

Review and Digression on Probability Distributions

Let us now extend some of our earlier discussions (Chapter 5). In general we have

$$\left\langle \hat{R} \right\rangle = Tr\left(\hat{\rho}\hat{R}\right) \tag{15.123}$$

Now if g(r)dr is the probability that the observable R lies between r and r + dr, then by definition

$$\left\langle F(\hat{R})\right\rangle = \int_{-\infty}^{\infty} F(r')g(r')dr' = Tr\left(\hat{\rho}F(\hat{R})\right)$$
(15.124)

Let us now extract the probability density g(r) using these results.

Discrete Spectrum

Let \hat{R} have a purely discrete spectrum. We can then write

$$\hat{R} = \sum_{n} r_{n} \left| r_{n} \right\rangle \left\langle r_{n} \right| \tag{15.125}$$

Now consider the function

$$F(R) = \theta(r - R) = \begin{cases} 1 & R < r \\ 0 & R > r \end{cases}$$
(15.126)

We then have

$$\left\langle \theta(r - \hat{R}) \right\rangle = \int_{-\infty}^{r} g(r') dr' = \Pr ob(R < r|\rho)$$

$$= Tr \left(\hat{\rho} \theta(r - \hat{R}) \right)$$

$$= Tr \left[\hat{\rho} \left(\sum_{n} \theta(r - r_{n}) |r_{n}\rangle \langle r_{n}| \right) \right]$$

$$= \sum_{n} \theta(r - r_{n}) \langle r_{n}| \hat{\rho} |r_{n}\rangle$$
(15.127)

Therefore,

$$g(r) = \frac{\partial}{\partial r} \operatorname{Pr} ob(R < r|\rho)$$

= $\frac{\partial}{\partial r} \sum_{n} \theta(r - r_{n}) \langle r_{n} | \hat{\rho} | r_{n} \rangle$
= $\sum_{n} \delta(r - r_{n}) \langle r_{n} | \hat{\rho} | r_{n} \rangle$ (15.128)

This makes it clear that g(r) = 0 if r is not an eigenvalue.

The probability that R will have the discrete value r in the virtual ensemble characterized by $\hat{\rho}$ is

$$Prob(R = r|\rho) = \lim_{\varepsilon \to 0} \left[Prob(R < r + \varepsilon|\rho) - Prob(R < r - \varepsilon|\rho) \right]$$
$$= \sum_{n} \delta_{r,r_{n}} \langle r_{n} | \hat{\rho} | r_{n} \rangle$$
(15.129)

If we define the projection operator

$$\hat{P}(r) = \sum_{n} |r_n\rangle \langle r_n | \delta_{r, r_n}$$
(15.130)

which projects onto the subspace spanned by all the degenerate eigenvectors with eigenvalue $r = r_n$. We then have

$$Prob(R = r|\rho) = Tr\left(\hat{\rho}\hat{P}(r)\right)$$
(15.131)

In the special case of a pure state where $\hat{\rho} = |\psi\rangle \langle \psi|$ and a non-degenerate eigenvalue, this reduces to

$$\operatorname{Prob}(R = r_n | \rho) = \left| \langle r_n | \psi \rangle \right|^2 \tag{15.132}$$

A particular dynamical variable will, in general, have a non-vanishing statistical dispersion in most states. In the case of a discrete variable, however, it is possible for all of the probability to be concentrated on a single value. If the dynamical variable R takes on the unique value r_0 (assumed to be a non-degenerate eigenvalue) with probability = 1 in some state, then from

$$Prob(R = r|\rho) = \sum_{n} \delta_{r,r_n} \langle r_n | \hat{\rho} | r_n \rangle$$
(15.133)

we must have

$$\langle r_0 | \hat{\rho} | r_0 \rangle = 1 \tag{15.134}$$

But, any state operator must satisfy $Tr\hat{\rho}^2 \leq 1$ which implies

$$\sum_{m,n} \langle r_n | \hat{\rho} | r_m \rangle \langle r_m | \hat{\rho} | r_n \rangle = \sum_{m,n} \left| \langle r_n | \hat{\rho} | r_m \rangle \right|^2 \le 1$$
(15.135)

Since one term in the sum already accounts for an amount = 1, all of the other diagonal and non-diagonal matrix elements of $\hat{\rho}$ must vanish.

Therefore the only state for which R takes on the non-degenerate eigenvalue r_0 with probability = 1 is the pure state $\hat{\rho} = |r_0\rangle \langle r_0|$. This is what we mean by an eigenstate.

Continuous Spectrum

Let \hat{Q} be a Hermitian operator having a purely continuous spectrum such that

$$\hat{Q}|q'\rangle = q'|q'\rangle \tag{15.136}$$

Then we can write

$$\hat{Q} = \int q' |q'\rangle \langle q'| \, dq' \tag{15.137}$$

The eigenvectors are normalized by the relation

$$\langle q' \mid q'' \rangle = \delta(q' - q'') \tag{15.138}$$

Now let g(q)dq be the probability that the corresponding observable Q lies between q and q + dq. We then get

$$\left\langle \theta(q - \hat{Q}) \right\rangle = \int_{-\infty}^{q} g(q') dq' = \Pr ob(Q < q|\rho)$$

$$= Tr \left(\hat{\rho} \theta(q - \hat{Q}) \right) = Tr \left[\hat{\rho} \int_{-\infty}^{\infty} \theta(q - q') |q'\rangle \langle q'| dq' \right]$$

$$= \int_{-\infty}^{q} \langle q'| \hat{\rho} |q'\rangle dq'$$
(15.139)

or

$$g(q) = \frac{\partial}{\partial q} \operatorname{Pr} ob(Q < q|\rho) = \langle q| \hat{\rho} |q\rangle$$
(15.140)

Once again in the pure state we get

$$g(q) = \left| \left\langle q \mid \psi \right\rangle \right|^2 \tag{15.141}$$

The expressions for the probability and the probability density always consist of a relation between two factors: one characterizing the state (the state function) and one characterizing a portion of the spectrum being observed(the filter function).

In the expression

$$Prob(R = r|\rho) = Tr\left(\hat{\rho}\hat{P}(r)\right)$$
(15.142)

they are $\hat{\rho}$ and $\hat{P(r)}$ respectively.

In the expressions $|\langle r_n | \psi \rangle|^2$ and $|\langle q | \psi \rangle|^2$ they are the state vector ψ and an eigenvector belonging to the observable.

The two objects have very distinct natures, i.e., the state vector must be normalized and therefore belongs to Hilbert space. The filter function does not necessarily belong to Hilbert space, but rather to an extended or *rigged Hilbert* space.

Returning to our discussion, we have the following situation. Associated with any dynamical variable R and its corresponding Hermitian operator \hat{R} is a family of projection operators $M_R(\Delta)$ which are related to the eigenvectors and eigenvalues of \hat{R} by

$$M_R(\Delta) = \sum_{r_n \in \Delta} |r_n\rangle \langle r_n| \qquad (15.143)$$

The sum is over all eigenvectors (even degenerate) whose eigenvalues lie in the subset Δ . For a continuous spectrum the sum becomes an integral. Then the probability that the value of R will lie within Δ is given by

$$Prob(R \in \Delta | \rho) = Tr\left(\hat{\rho}M_R(\Delta)\right) \tag{15.144}$$

If the region Δ contains only one eigenvalue, then this reduces the earlier result for $Prob(R = r|\rho)$ and in the continuous spectrum case it is equal to the integral of the probability density over the region Δ . This result satisfies all of the 4 probability axioms in Chapter 5.

We then have

$$Prob(A|C) = Prob(R \in \Delta_a|\rho) = Tr(\hat{\rho}M_R(\Delta_a))$$
(15.145)

The joint probability $Prob(A \wedge B|C)$ can be evaluated only if we can find(from quantum mechanics) a projection operator for the compound event $A \wedge B$. This is possible if the projection operators $M_R(\Delta_a)$ and $M_S(\Delta_b)$ commute. In that case the product $M_R(\Delta_a)M_S(\Delta_b)$ is also a projection operator that projects onto the subspace spanned by those common eigenvectors of \hat{R} and \hat{S} with eigenvalues in the ranges Δ_a and Δ_b , respectively. We then have

$$Prob(A \land B|C) = Prob\left((R \in \Delta_a) \land (S \in \Delta_b)|\rho\right)$$
$$= Tr\left(\hat{\rho}M_R(\Delta_a)M_S(\Delta_b)\right)$$
(15.146)

This is just the joint probability that both events A and B occur on the condition C, or, in other words, it is the probability that the result of the measurement of R at time t_a is in the range Δ_a and the result of the measurement of S at time t_b is in the range Δ_b , following the state preparation corresponding to $\hat{\rho}$. If \hat{R} and \hat{S} commute this calculation is possible for arbitrary ranges.

The last term $Prob(B|A \wedge C)$ is

$$Prob(B|A \wedge C) = Prob\left((S \in \Delta_b)|(R \in \Delta_a) \wedge \rho\right)$$
(15.147)

It is the probability for a result of the S measurement, conditional on the state preparation and a certain result of the R measurement. We do not know how to deal with these expressions directly.

Two paths are now open to us.

- 1. We can regard the preparation of the state $\hat{\rho}$ and the following measurement of R as a composite operation that corresponds to the preparation of a new state $\hat{\rho}'$.
- 2. We can define

$$Prob(B|A \wedge C) = \frac{Prob(A \wedge B|C)}{Prob(A|C)}$$
(15.148)

since we know how to calculate the right-hand-side.

Filtering-Type Measurements

If we want to regard the initial ρ - state preparation followed by the R measurement as a composite operation that results in a new state ρ' , then we require a detailed description of the R measurement apparatus and a dynamical analysis of its operation. This is only possible for particular cases and no general treatment can be done.

Are there any types of measurements that we can treat without too much difficulty?

Let us consider a measurement of the filtering type where the ensemble of systems generated by the ρ - state preparation is separated into sub-ensembles according to the value of the dynamical variable R (SG apparatus is an example of this type of measurement).

If we consider the result of a subsequent S measurement on only that subensemble for which $R \in \Delta_a$, and ignore the rest, then we are determining the conditional probability

$$Prob(B|A\&C) = Prob((S \in \Delta_b)|(R \in \Delta_a) \land \rho)$$
(15.149)

This filtering process, which has the effect of removing all values of R except those for which $R \in \Delta_a$, can be regarded as preparing a new state that is represented by

$$\hat{\rho}' = \frac{M_R(\Delta_a)\hat{\rho}M_R(\Delta_a)}{Tr\left[M_R(\Delta_a)\hat{\rho}M_R(\Delta_a)\right]}$$
(15.150)

so that we have

$$Prob(B|A \land \rho) = Prob((S \in \Delta_b) | (R \in \Delta_a) \land \rho)$$

=
$$Prob((S \in \Delta_b) | \rho') = Tr(\rho' M_S(\Delta_b))$$
(15.151)

Finally, we can calculate a joint probability for two filtering-type measurements as:

$$Prob(A \wedge B|C) = \Pr ob(A|C) \Pr ob(B|A \wedge C)$$

$$= \Pr ob(A|\rho) \Pr ob(B|A \wedge \rho)$$

$$= Tr(\hat{\rho}M_{R}(\Delta_{a})) Tr(\hat{\rho}'M_{S}(\Delta_{b}))$$

$$= Tr(\hat{\rho}M_{R}(\Delta_{a})) Tr\left(\frac{M_{R}(\Delta_{a})\hat{\rho}M_{R}(\Delta_{a})}{Tr[M_{R}(\Delta_{a})\hat{\rho}M_{R}(\Delta_{a})]}M_{S}(\Delta_{b})\right)$$

$$= \frac{Tr(\hat{\rho}M_{R}(\Delta_{a}))}{Tr[M_{R}(\Delta_{a})\hat{\rho}M_{R}(\Delta_{a})]}Tr(M_{R}(\Delta_{a})\hat{\rho}M_{R}(\Delta_{a})M_{S}(\Delta_{b}))$$

$$= \frac{Tr(\hat{\rho}M_{R}(\Delta_{a}))}{Tr[\hat{\rho}M_{R}(\Delta_{a})M_{R}(\Delta_{a})]}Tr(\hat{\rho}M_{R}(\Delta_{a})M_{S}(\Delta_{b})M_{R}(\Delta_{a}))$$

$$= \frac{Tr(\hat{\rho}M_{R}(\Delta_{a}))}{Tr[\hat{\rho}M_{R}(\Delta_{a})]}Tr(\hat{\rho}M_{R}(\Delta_{a})M_{S}(\Delta_{b})M_{R}(\Delta_{a}))$$

$$= Tr(\hat{\rho}M_{R}(\Delta_{a})]$$
(15.152)

In the case when $M_R(\Delta_a)$ and $M_S(\Delta_b)$ commute, this reduces to the earlier expression

$$Prob(A \wedge B|C) = Tr\left(\hat{\rho}M_R(\Delta_a)M_S(\Delta_b)\right)$$
(15.153)

The derivation of this last relation required that \hat{R} and \hat{S} commute, but no such restriction was required to derive

$$Prob(B|A \wedge \rho) = Tr\left(\rho' M_S(\Delta_b)\right) \tag{15.154}$$

The latter, however, is restricted to filtering-type measurements.

We have just seen that both results are consistent with

$$Prob(A \land B|C) = Prob(A|C)Prob(B|A \land C)$$
(15.155)

when all the various conditions are satisfied together. It does seem strange however that the conditions for evaluating the two sides of the equation should be different. This is not really a puzzle, however.

The derivation of $Prob(A \land B|C)$ was implicitly based on the assumption that the measurements of R and S were equivalent to, or at least compatible with, *a joint filtering according to the eigenvalues of* R and S, i.e., a product of projection operators. This is only possible if R and S commute. In this case the time order of measurements is irrelevant, as is clear from the symmetry with respect to the two projection operators, i.e.,

$$Prob(A \wedge B|C) = Tr\left(\hat{\rho}M_R(\Delta_a)M_S(\Delta_b)\right)$$
(15.156)

Remember these are time-dependent operators in the Heisenberg picture.

If the operators R and S do not commute, the above relation is not true, as the definition of the joint probability. In this case we must carefully observe the time orderings, because it is the R measurement that serves as (part of the) state preparation for the S measurement and not vice versa. This is clear in the lack of symmetry in the last result

$$Prob(A \wedge B|C) = Tr\left(\hat{\rho}M_R(\Delta_a)M_S(\Delta_b)M_R(\Delta_a)\right)$$
(15.157)

Application to Spin Measurements

Let us now illustrate these ideas in a spin = 1/2 system.

Assume a state represented by $|\psi\rangle$ has been prepared. It is then subjected to three successive measurements of the filtering type:

a measurement of $\hat{\sigma}_z$ at time t_1 a measurement of $\hat{\sigma}_u$ at time t_2 a measurement of $\hat{\sigma}_x$ at time t_3

where the *u*-direction is in the zx-plane, making an angle θ with respect to the *z*-axis. These filtering measurements will split the initial beam first into two, then into four, and finally into eight separated subbeams as in Figure 15.7 below:



Figure 15.7: Filtering Splitting Beam

Seven SG machines are required to carry out this experiment. We assume that the spin vector is a constant of the motion between the measurements.

Each of the eight final outcomes of this experiment corresponds to a particular combination of results (+1 or -1) for the three $(\hat{\sigma}_z, \hat{\sigma}_u, \hat{\sigma}_x)$ measurements, and the probability of these various outcomes is, in fact, the *joint probability* for the results of the three measurements.

The full notation for this joint probability should be

$$Prob(\hat{\sigma}_z = a, \hat{\sigma}_u = b, \hat{\sigma}_x = c | \psi \wedge X)$$
(15.158)

with $a = \pm 1$, $b = \pm 1$ and $c = \pm 1$. As indicated above, the probability is conditional on the state preparation (denoted by ψ) and the configuration of the SG

machines (denoted by X). We abbreviate it $Prob(a, b, c | \psi \wedge X)$ with the time ordering assumed.

It is important to note that this is the joint probability for the results of three actual measurements, and not the joint distribution for hypothetical simultaneous values of three noncommuting observables. Moreover, the various subbeams in this experiment are all separated in space and no attempt is made to recombine them. Thus, questions of relative phase and coherence are irrelevant.

We write the initial state vector as

$$|\psi\rangle = \alpha |z+\rangle + \beta |z-\rangle \tag{15.159}$$

in the basis of the $\hat{\sigma}_z$ eigenvectors. The amplitudes are divided at each filtering operation and the division is calculated using projection operators. The absolute squares of these amplitudes then give the probabilities of the various measurements.

After the measurement of $\hat{\sigma}_z$ at t_1 we have

$$P_{z}(a|\psi\&X) = \langle \psi | M_{z}(a) | \psi \rangle$$

= $\langle \psi | (|a\rangle \langle a|) | \psi \rangle = |\langle a | \psi \rangle|^{2}$
=
$$\begin{cases} |\alpha|^{2} & \text{for } a = +1 \text{ or } |a\rangle = |z+\rangle \\ |\beta|^{2} & \text{for } a = -1 \text{ or } |a\rangle = |z-\rangle \end{cases}$$
(15.160)

Similarly, after the measurement of $\hat{\sigma}_u$ at t_2 we have

$$P_{zu}(a,b|\psi \wedge X) = \left(\langle \psi | \hat{M}_z(a) \rangle \hat{M}_u(b) \left(\hat{M}_z(a) | \psi \rangle \right) \\ = \langle \psi | \hat{M}_z(a) \hat{M}_u(b) \hat{M}_z(a) | \psi \rangle$$
(15.161)

where

$$\hat{M}_u(\pm 1) = |u\pm\rangle\langle u\pm| \tag{15.162}$$

and

$$|u+\rangle = \cos\frac{\theta}{2}|z+\rangle + \sin\frac{\theta}{2}|z-\rangle \quad , \quad |u-\rangle = -\sin\frac{\theta}{2}|z+\rangle + \cos\frac{\theta}{2}|z-\rangle$$
 (15.163)

Finally after the measurement of $\hat{\sigma}_x$ at t_3 we have

$$P_{zu}(a, b, c | \psi \wedge X) = (\langle \psi | \hat{M}_{z}(a) \hat{M}_{u}(b)) \hat{M}_{x}(c) (\hat{M}_{u}(b) \hat{M}_{z}(a) | \psi \rangle) = \langle \psi | \hat{M}_{z}(a) \hat{M}_{u}(b) \hat{M}_{x}(c) \hat{M}_{u}(b) \hat{M}_{z}(a) | \psi \rangle$$
(15.164)

Now we can always write

$$P_{zu}(a,b|\psi \wedge X) = \sum_{c=\pm 1} P_{zu}(a,b,c|\psi \wedge X)$$
(15.165)

i.e., the probability for the z and u measurements independent of what happens at the x measurement (the later x measurement should not affect them!).

We then get

$$P_{zu}(a, b|\psi \wedge X) = \sum_{c=\pm 1} P_{zux}(a, b, c|\psi \wedge X)$$

$$= \sum_{c=\pm 1} \langle \psi | \hat{M}_{z}(a) \hat{M}_{u}(b) \hat{M}_{x}(c) \hat{M}_{u}(b) \hat{M}_{z}(a) |\psi \rangle$$

$$= \langle \psi | \hat{M}_{z}(a) \hat{M}_{u}(b) (\hat{M}_{x}(c=+1) + \hat{M}_{x}(c=-1)) \hat{M}_{u}(b) \hat{M}_{z}(a) |\psi \rangle$$

$$= \langle \psi | \hat{M}_{z}(a) \hat{M}_{u}(b) \hat{M}_{u}(a) |\psi \rangle$$

$$= \langle \psi | \hat{M}_{z}(a) \hat{M}_{u}(b) \hat{M}_{z}(a) |\psi \rangle$$
(15.166)

as expected.

So the presence of the $\hat{\sigma}_x$ filter has no effect on the earlier measurements. Similarly, we have

$$P_{z}(a|\psi \wedge X) = \sum_{b=\pm 1} \sum_{c=\pm 1} P_{zux}(a, b, c|\psi \wedge X)$$
$$= \langle \psi | \hat{M}_{z}(a) |\psi \rangle$$
(15.167)

since the absence of the $\hat{\sigma}_x$ and $\hat{\sigma}_u$ filters has no effect on the measurement of $\hat{\sigma}_z$.

Now several interesting conditional probabilities can be calculated from these joint probability distributions using the formula

$$Prob(B|A \wedge C) = \frac{Prob(A \wedge B|C)}{Prob(A|C)}$$
(15.168)

(1) Conditioning on a Prior Measurement

Let C be the preparation of the state ψ , A be the result $\hat{\sigma}_z = +1$ for the first measurement, and B be to result of the measurement of $\hat{\sigma}_u$. Then the probability that the second measurement will yield $\hat{\sigma}_u = +1$ conditional on both the state preparation and the result $\hat{\sigma}_z = +1$ in the first measurement is

$$Prob(\hat{\sigma}_{u} = +1 | (\hat{\sigma}_{z} = +1) \land \psi) = \frac{P_{zu}(+1, +1 | \psi)}{P_{z}(+1 | \psi)}$$
$$= \frac{\langle \psi | \hat{M}_{z}(+1) \hat{M}_{u}(+1) \hat{M}_{z}(+1) | \psi \rangle}{\langle \psi | \hat{M}_{z}(+1) | \psi \rangle}$$
$$= \frac{|\alpha \cos \frac{\theta}{2}|^{2}}{|\alpha|^{2}} = \cos^{2} \frac{\theta}{2}$$
(15.169)

This is the same as the probability of obtaining $\hat{\sigma}_u = +1$ conditional on the new state being $|\psi'\rangle = |z+\rangle$, i.e., as if the first measurement collapsed or reduced the state to correspond to the measurement. We have not, however, assumed any reduction process. This result follows from existing quantum mechanical rules. It does not, however, say that any collapse occurred!

(2) Probability Distribution for $\hat{\sigma}_x$ regardless of $\hat{\sigma}_z$ and $\hat{\sigma}_u$

The probability of the result $\hat{\sigma}_x = +1$ in the final measurement regardless of the results of the prior measurements is

$$P_{x}(+1|\psi \wedge X) = \sum_{a=\pm 1} \sum_{b=\pm 1} P(a, b, +1|\psi \wedge X)$$

=
$$\sum_{a=\pm 1} \sum_{b=\pm 1} \langle \psi | \hat{M}_{z}(a) \hat{M}_{u}(b) \hat{M}_{x}(+1) \hat{M}_{u}(b) \hat{M}_{z}(a) |\psi \rangle \quad (15.170)$$

Now

$$P(a,b,c|\psi \wedge X) = \langle \psi | \hat{M}_z(a) \hat{M}_u(b) \hat{M}_x(c) \hat{M}_u(b) \hat{M}_z(a) | \psi \rangle$$
(15.171)

or

$$P(+1,+1,+1|\psi \wedge X) = \frac{1}{2} |\alpha|^2 \cos^2 \frac{\theta}{2} [1+\sin\theta]$$
(15.172)

$$P(-1,+1,+1|\psi \wedge X) = \frac{1}{2} |\beta|^2 \sin^2 \frac{\theta}{2} [1+\sin\theta]$$
(15.173)

$$P(+1, -1, +1|\psi \wedge X) = \frac{1}{2} |\alpha|^2 \sin^2 \frac{\theta}{2} [1 - \sin \theta]$$
(15.174)

$$P(-1, -1, +1|\psi \wedge X) = \frac{1}{2} |\beta|^2 \cos^2 \frac{\theta}{2} [1 - \sin \theta]$$
(15.175)

and therefore carrying out the sum we get

$$P_x(+1|\psi \wedge X) = \frac{1}{2} \left[1 + (|\alpha|^2 - |\beta|^2) \sin \theta \cos \theta \right]$$
(15.176)

This is the probability of obtaining the result $\hat{\sigma}_x = +1$ with the $\hat{\sigma}_z$ and $\hat{\sigma}_u$ filters in place, but ignoring the results of the $\hat{\sigma}_z$ and $\hat{\sigma}_u$ measurements. It is *not* equal to the probability of obtaining $\hat{\sigma}_x = +1$ with the $\hat{\sigma}_z$ and $\hat{\sigma}_u$ filters absent, which is

$$P_x(+1|\psi) = \langle \psi | M_x(+1) | \psi \rangle \frac{1}{2} | \alpha + \beta |^2$$
(15.177)

These two results differ because the particle must pass through the $\hat{\sigma}_z$ and $\hat{\sigma}_u$ filters before reaching the $\hat{\sigma}_x$ filter and clearly the presence of the other filters is relevant!

Thus, we must always explicitly take the dynamical action of the apparatus into account when developing a theory of measurement.

(3) Conditioning on Both Earlier and Later Measurements

We now calculate the probability for a particular result of the intermediate $\hat{\sigma}_u$ measurement, conditional on specified results for the *preceding* $\hat{\sigma}_z$ measurement and the *following* $\hat{\sigma}_x$ measurement.

The later measurement cannot have any *causal* effect on the outcome of the earlier measurement, but it can give relevant information because of the *statistical correlations* between the results of successive measurements!

We use

$$Prob(B|A \wedge C) = \frac{Prob(A \wedge B|C)}{Prob(A|C)}$$
(15.178)

with $C = \psi \wedge X$, $A = (\hat{\sigma}_z(t_1) = +1) \wedge (\hat{\sigma}_x(t_3) = +1)$ and $B = (\hat{\sigma}_u(t_2) = +1)$. We get

$$Prob((\hat{\sigma}_{u}(t_{2}) = +1)|(\hat{\sigma}_{z}(t_{1}) = +1) \land (\hat{\sigma}_{x}(t_{3}) = +1) \land \psi \land X)$$
$$= \frac{P(+1, +1, +1|\psi \land X)}{P_{zx}(+1, +1|\psi \land X)}$$
(15.179)

From earlier we have

$$P(+1,+1,+1|\psi \wedge X) = \frac{1}{2} |\alpha|^2 \cos^2 \frac{\theta}{2} [1+\sin \theta]$$
 (15.180)

and

$$P_{zx}(+1,+1|\psi\&X) = P(+1,+1,+1|\psi\land X) + P(+1,-1,+1|\psi\land X)$$
$$= \frac{1}{2} |\alpha|^2 \cos^2 \frac{\theta}{2} [1+\sin \theta] + \frac{1}{2} |\alpha|^2 \sin^2 \frac{\theta}{2} [1-\sin \theta]$$
$$= \frac{1}{2} |\alpha|^2 (1+\sin \theta \cos \theta)$$
(15.181)

Putting it all together we get

$$Prob((\hat{\sigma}_u(t_2) = +1)|(\hat{\sigma}_z(t_1) = +1) \land (\hat{\sigma}_x(t_3) = +1) \land \psi \land X)$$
$$= \left(\cos^2 \frac{\theta}{2}\right) \frac{1 + \sin \theta}{1 + \sin \theta \cos \theta}$$
(15.182)

Thus, the probability distribution for $\hat{\sigma}_u$ is well-defined for all θ . There is , however, no quantum state $\hat{\rho}'$ such that

$$Prob(\hat{\sigma}_u = +1|\rho') = \left(\cos^2\frac{\theta}{2}\right) \frac{1+\sin\theta}{1+\sin\theta\cos\theta}$$
(15.183)

This is clear from the fact that

$$Prob((\hat{\sigma}_u(t_2) = +1) | (\hat{\sigma}_z(t_1) = +1) \land (\hat{\sigma}_x(t_3) = +1) \land \psi \land X) = 1$$
(15.184)

i.e., the probability is 1 for both $\theta = 0$ and $\theta = \pi/2$, which is very different than case (1).

How do we resolve this paradox?

We must remember that a quantum state is characterized by a *well-defined* state preparation procedure that can yield a statistically reproducible ensemble of systems, and not merely by the specification of abstract information.

This is why the probabilities in these examples have been conditional on the apparatus configuration X.

Now the angle θ specifies the direction of the $\hat{\sigma}_u$ filter and it must be included in X, i.e., we should write X_{θ} . By conditioning on the final result $\hat{\sigma}_x = +1$ we select a subensemble discarding those cases in which the result is -1. However, a part of the specification of this subensemble is that its members have passed through the $\hat{\sigma}_u$ filter. Thus, the conditions that define the subensemble include the value of the angle θ , which therefore may not be changed.

In the usual situation, as in case (1), all of the specifications correspond to operations performed before the measurement of interest. Hence, they define an ensemble whose composition does not depend upon what measurement we may choose to perform. We then have a well-defined state, which yields a welldefined probability distribution for any subsequent measurement that we may choose to perform.

But this is not possible if we specify conditional information both before and after the measurement of interest, as in the last example.

Thus, the paradox is resolved and makes us realize that we must pay very careful attention to the state preparation concepts.

Comparing Approaches

Let us now look at all of this theory in a more standard manner (as is done in many textbooks) and then compare the two approaches.

The standard axioms of quantum theory are:

- 1. The state is described by a vector $|\psi\rangle$ in a linear space.
- 2. The observables are represented by Hermitian operators and a function of an observable f(observable) is represented by f(operator).
- 3. The expectation value of an observable is $\langle \psi | operator | \psi \rangle$.

4. The dynamics are given by the Schrodinger equation

0

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$
 where \hat{H} = Hamiltonian or energy operator

- 5. The only possible results of a measurement of an observable are the eigenvalues of the corresponding operator.
- 6. In a measurement of the observable \hat{A} with the result a, the original state changes into state $|a\rangle$ where

$$\hat{A}|a\rangle = a|a\rangle$$

In this text, we made a different set of assumptions:

Postulate 1

For each dynamical variable or observable, which is a physical concept, there corresponds a Hermitian, linear operator, which is a mathematical object.

The possible values of any measurement of the observable are restricted to the eigenvalues of the corresponding operator.

Postulate 1 is equivalent to axioms (2) and (5).

Postulate 2

- (a) A density operator exists for every real physical system.
- (b) The expectation value of an operator \hat{B} is given by

$$\langle \hat{B} \rangle = Tr(\hat{W}\hat{B})$$

Postulate 2 is equivalent to axioms (1) and (3).

We also assumed that we were in a linear vector space and hence could prove Stone's theorem which is equivalent to axiom (4) above.

We did not assume axiom (6).

In the discussion just completed we saw that axiom (6) seems to be incorporated in our theory but is not generally true.

It is at the heart of all the controversy in quantum mechanics.

Let us see how the standard approach proceeds.

First, both approaches imply that if a system is in the state (linear combination)

$$|\psi\rangle = \sum_{n} c_n |a_n\rangle \text{ where } \hat{A} |a_n\rangle = a_n |a_n\rangle$$
 (15.185)

then the probability during a measurement of A that we measure the eigenvalue a_m is given by

$$\left|\left\langle a_m \mid \psi\right\rangle\right|^2 = \left|c_n\right|^2 \tag{15.186}$$

The conceptual difficulties that we will elucidate within the structure of the quantum mechanical state do not imply a weakness in quantum theory, whose experimental validity has never encountered any limitations, but only a weakness of our imagination!!

The Density Matrix in the Standard Approach

Pure and Mixed Ensembles

If a system is in a state $|\psi\rangle$, then the observable \hat{A} has the average or expectation value

$$\left\langle \hat{A} \right\rangle = \left\langle \psi \right| \hat{A} \left| \psi \right\rangle \tag{15.187}$$

If we define a new operator called the density operator given by

$$\hat{\rho} = |\psi\rangle\langle\psi| \tag{15.188}$$

then we have these properties

$$Tr(\hat{\rho}\hat{A}) = \sum_{n} \langle n|\hat{\rho}\hat{A}|n\rangle = \sum_{n} \langle n|\psi\rangle \langle \psi|\hat{A}|n\rangle$$
$$= \sum_{n} \langle \psi|\hat{A}|n\rangle \langle n|\psi\rangle = \langle \psi|\hat{A}\hat{I}|\psi\rangle = \langle \psi|\hat{A}|\psi\rangle$$
(15.189)

$$Tr(\hat{\rho}) = Tr(\hat{\rho}\hat{I}) = \langle \psi | \hat{I} | \psi \rangle = \langle \psi | \psi \rangle = 1$$
(15.190)

$$\hat{\rho}^{2} = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho}$$
(15.191)

If we let $\{|n\}$ and $\{|m\}$ be two different basis systems, then we have

$$Tr(\hat{X}) = \sum_{n} \langle n | \hat{X} | n \rangle = \sum_{n,m} \langle n | m \rangle \langle m | \hat{X} | n \rangle$$
$$= \sum_{n,m} \langle m | \hat{X} | n \rangle \langle n | m \rangle = \sum_{m} \langle m | \hat{X} | m \rangle$$

so that the trace is independent of the basis.

If the systems or objects under investigation are all in one and the same state $|\psi\rangle$, we call this a *pure ensemble* or we say that the system is in a *pure state*.

In order to verify the probability predictions contained in the state vector $|\psi\rangle$ experimentally , we must , in fact, investigate an ensemble of identically prepared objects. If

$$|\psi\rangle = \sum_{n} c_n |n\rangle \tag{15.192}$$

then the eigenvalue a_n will be the \hat{A} measurement result N_n times for an ensemble of N objects. The larger N, the more precisely N_n/N approaches the probability $|c_n|^2$, i.e.,

$$\left|c_{n}\right|^{2} = \lim_{N \to \infty} \frac{N_{n}}{N} \tag{15.193}$$

and the expectation value correspondingly becomes

$$\left\langle \hat{A} \right\rangle = \sum_{n} \left| c_n \right|^2 a_n = \lim_{N \to \infty} \frac{1}{N} \sum_{n} N_n a_n \tag{15.194}$$

In addition to the inherent statistical character residing in the states themselves, an ensemble can also contain a statistical distribution of states.

If an ensemble with distinct states is present, we call this a mixed ensemble, a mixture, or we say a mixed state. Suppose that of the N representatives of the ensemble, N_1 are in the state $|\psi_1\rangle$, N_2 are in the state $|\psi_2\rangle$, etc. Then the probability that an arbitrarily chosen element of the ensemble is in the state $|\psi_i\rangle$ is given by

$$p_i = \frac{N_i}{N} \to \sum_i p_i = \sum_i \frac{N_i}{N} = \frac{1}{N} \sum_i N_i = 1$$
 (15.195)

The expectation value of \hat{A} is then

$$\left\langle \hat{A} \right\rangle = \sum_{n} p_i \left\langle \psi_i \right| \hat{A} \left| \psi_i \right\rangle \tag{15.196}$$

This expectation value can also be represented by a density matrix of the form

$$\hat{\rho} = \sum_{i} p_i |\psi_i\rangle \langle\psi_i| \tag{15.197}$$

with the properties

$$Tr\left(\hat{\rho}\hat{A}\right) = \sum_{n} \langle n|\hat{\rho}\hat{A}|n\rangle = \sum_{n,i} p_{i} \langle n|\psi_{i}\rangle \langle \psi_{i}|\hat{A}|n\rangle$$
$$= \sum_{n,i} p_{i} \langle \psi_{i}|\hat{A}|n\rangle \langle n|\psi_{i}\rangle = \sum_{i} p_{i} \langle \psi_{i}|\hat{A}|\psi_{i}\rangle = \langle \hat{A}\rangle$$
(15.198)

$$Tr\left(\hat{\rho}\right) = 1 \tag{15.199}$$

$$\hat{\rho}^{2} = \sum_{i,j} p_{i} p_{j} |\psi_{i}\rangle \langle\psi_{i} |\psi_{j}\rangle \langle\psi_{j}| \neq \hat{\rho}$$
(15.200)

For each $|\psi\rangle$

$$\langle \psi | \hat{\rho} | \psi \rangle = \sum_{i} p_{i} |\langle \psi | \psi_{i} \rangle|^{2} \ge 0 \rightarrow non - negative$$
 (15.201)

If

$$\hat{\rho}|m\rangle = P_m|m\rangle \rightarrow \hat{\rho} = \sum_m P_m|m\rangle\langle m|$$
 (15.202)

then

$$\langle \psi | \hat{\rho} | \psi \rangle = \sum_{m} P_m \left| \langle m | \psi \rangle \right|^2 \ge 0 \rightarrow P_m \ge 0$$
 (15.203)

and

$$\sum_{m} P_{m} = \sum_{m} \langle m | \hat{\rho} | m \rangle = \sum_{m} \langle m | \left(\sum_{i} p_{i} | \psi_{i} \rangle \langle \psi_{i} | \right) | m \rangle$$
$$= \sum_{i} p_{i} \sum_{m} |\langle m | \psi_{i} \rangle|^{2} = 1$$

We also have

$$\hat{\rho}^2 = \sum_m P_m^2 |m\rangle \langle m| \to Tr \hat{\rho}^2 = \sum_m P_m^2 < 1$$
 (15.204)

Thus, the criterion for a pure state is $Tr\hat{\rho}^2$ = 1 and for a mixed state $Tr\hat{\rho}^2 < 1.$

Now the expectation value of the projection operator $|n\rangle \langle n|$ (discrete spectrum) is given by

$$Tr(|n\rangle \langle n|\hat{\rho}) = \sum_{i} p_{i} |\langle n|\psi_{i}\rangle|^{2} = \sum_{i} p_{i} |c_{n}^{(i)}|^{2}$$
(15.205)

which is equal to the probability of obtaining the state $|n\rangle$ as a result of a measurement.

The expectation value of the projection operator $|x\rangle\langle x|$ (continuous spectrum) is given by

$$Tr(|x\rangle\langle x|\hat{\rho}) = \sum_{i} p_{i} |\langle x|\psi_{i}\rangle|^{2} = \sum_{i} p_{i} |\psi_{i}(x)|^{2}$$
(15.206)

which is equal to the probability of obtaining the state $|x\rangle$ as a result of a measurement.

Now let us consider a system consisting of two subsystems 1 and 2 with orthonormal basis states $\{|1n\rangle\}$ and $\{|2n\rangle\}$, respectively. A general pure state in the direct product space is then

$$|\psi\rangle = \sum_{m,n} c_{nm} |1n\rangle |2m\rangle$$
 where $\sum_{n,m} |c_{nm}|^2 = 1$ (15.207)

The corresponding density operator is

$$\hat{\rho} = |\psi\rangle \langle \psi| = \sum_{n,m} \sum_{n'.m'} c_{nm} c_{n'm'}^* |1n\rangle |2m\rangle \langle 1n'| \langle 2m'|$$
(15.208)

If we carry out measurements concerning only subsystem 1, that is, if the operators corresponding to the observables being measured only act on the states $|1n\rangle$, then

$$\begin{split} \left\langle \hat{A} \right\rangle &= Tr\left(\hat{\rho}\hat{A}\right) = \sum_{m'',n''} \left\langle 2m'' \right| \left\langle 1n'' \right| \hat{\rho}\hat{A} \left| 1n'' \right\rangle \left| 2m'' \right\rangle \\ &= \sum_{m'',n''} \left\langle 2m'' \right| \left\langle 1n'' \right| \left(\sum_{n,m} \sum_{n'.m'} c_{nm} c^*_{n'm'} \left| 1n \right\rangle \left| 2m \right\rangle \left\langle 1n' \right| \left\langle 2m' \right| \right) \hat{A} \left| 1n'' \right\rangle \left| 2m'' \right\rangle \\ &= \sum_{m'',n''} \sum_{n,m} \sum_{n'.m'} c_{nm} c^*_{n'm'} \left(\left\langle 2m'' \right| \left\langle 1n'' \right| \right) \left(\left| 1n \right\rangle \left| 2m \right\rangle \right) \left\langle 1n' \right| \hat{A} \left| 1n'' \right\rangle \left\langle 2m' \right| \left\langle 2m'' \right\rangle \\ &= \sum_{m'',n''} \sum_{n,m} \sum_{n'.m'} c_{nm} c^*_{n'm'} \delta_{m,m''} \delta_{n,n''} \left\langle 1n' \right| \hat{A} \left| 1n'' \right\rangle \\ &= \sum_{n,n',m} c_{nm} c^*_{n'm} \left\langle 1n' \right| \hat{A} \left| 1n \right\rangle \end{split}$$

Now we can write

$$\sum_{n,n',m} c_{nm} c_{n'm}^* \langle 1n' | \hat{A} | 1n \rangle = \sum_{n''} \langle 1n'' | \left(\left(\sum_{n,n',m} c_{nm} c_{n'm}^* | 1n \rangle \langle 1n' | \right) \hat{A} \right) | 1n'' \rangle$$
$$= Tr_1 \left(\left(\sum_{n,n',m} c_{nm} c_{n'm}^* | 1n \rangle \langle 1n' | \right) \hat{A} \right) = Tr_1 \left(\hat{\rho} \hat{A} \right)$$

where

$$\hat{\bar{\rho}} = \sum_{n,n',m} c_{nm} c_{n'm}^* |1n\rangle \langle 1n'| = Tr_2 \hat{\rho} \to \text{appropriate density operator} \quad (15.209)$$

so that finally

$$\left\langle \hat{A} \right\rangle = Tr_1 \left[\left(Tr_2 \hat{\rho} \right) \hat{A} \right] \tag{15.210}$$

where Tr_k means trace over subsystem k. Now

$$\hat{\rho}^{2} = \sum_{n,n',m} c_{nm} c_{n'm}^{*} \sum_{n_{1},n'_{1},m_{1}} c_{n_{1}m_{1}} c_{n'_{1}m_{1}} |1n\rangle \langle 1n'| 1n_{1}\rangle \langle 1n'_{1}|$$

$$= \sum_{n,n',m} c_{nm} c_{n'm}^{*} \sum_{n_{1},n'_{1},m_{1}} c_{n_{1}m_{1}} c_{n'_{1}m_{1}}^{*} |1n\rangle \delta_{n'n_{1}} \langle 1n'_{1}|$$

$$= \sum_{n,n',n'_{1}} \left(\sum_{m} c_{nm} c_{n'm}^{*} \right) \left(\sum_{m_{1}} c_{n'm_{1}} c_{n'_{1}m_{1}}^{*} \right) |1n\rangle \langle 1n'_{1}|$$

which say that, in general

$$\hat{\rho}^2 \neq \hat{\bar{\rho}} \tag{15.211}$$

If, however, the c_{nm} take the form

$$c_{nm} = b_n d_m$$
 with $\sum_n |b_n|^2 = 1 = \sum_m |d_m|^2$ (15.212)

then we have

$$\begin{split} \hat{\rho}^{2} &= \sum_{n,n',n_{1}'} \left(\sum_{m} c_{nm} c_{n'm}^{*} \right) \left(\sum_{m_{1}} c_{n'm_{1}} c_{n_{1}'m_{1}}^{*} \right) |1n\rangle \langle 1n_{1}'| \\ &= \sum_{n,n',n_{1}'} \left(b_{n} b_{n'}^{*} \sum_{m} |d_{m}|^{2} \right) \left(b_{n'} b_{n_{1}'}^{*} \sum_{m_{1}} |d_{m_{1}}|^{2} \right) |1n\rangle \langle 1n_{1}'| \\ &= \sum_{n,n',n_{1}'} \left(b_{n} b_{n'}^{*} \right) \left(b_{n'} b_{n_{1}'}^{*} \right) |1n\rangle \langle 1n_{1}'| = \sum_{n,n',n_{1}'} b_{n} b_{n_{1}'}^{*} |1n\rangle \langle 1n_{1}'| \sum_{n'} |b_{n'}|^{2} \\ &= \sum_{n,n',n_{1}'} b_{n} b_{n_{1}'}^{*} |1n\rangle \langle 1n_{1}'| = \hat{\rho} \end{split}$$

In this case we have,

$$|\psi\rangle = \left(\sum_{n} b_n |1n\rangle\right) \left(\sum_{m} d_m |2m\rangle\right)$$
(15.213)

i.e., it is the direct product of two pure states of the subspaces 1 and 2.

It is also true, in this case, that

$$Tr_1\hat{\rho}^2 = \sum_{n,n'} \left(\sum_n c_{nm} c^*_{n'm} \right) \left(\sum_{m_1} c_{n_1m_1} c^*_{n'_1m_1} \right) = 1$$
(15.214)

Except for this special case, $\hat{\rho}$ represents the density operator of a mixed ensemble. If the information of a subspace is ignored, then the pure state becomes a mixed state.

Although the total system is in a pure state, the density operator $\hat{\rho}$, which yields all expectation values pertaining only to subsystem 1, represents a mixed ensemble in general.

Projection Operators

The projection operator in subspace 2, $|2m\rangle\,\langle 2m|$, projects onto the state $|2m\rangle.$ Therefore,

$$(|2m\rangle \langle 2m|) |\psi\rangle = |\psi\rangle = (|2m\rangle \langle 2m|) \sum_{m',n} c_{nm} |1n\rangle |2m'\rangle = \sum_{n} c_{nm} |1n\rangle |2m\rangle$$

and the state operator becomes

$$\hat{\rho} \to \frac{|2m\rangle \langle 2m| \,\hat{\rho} \, |2m\rangle \langle 2m|}{Tr_1 \langle 2m| \,\hat{\rho} \, |2m\rangle} \tag{15.215}$$

This implies that if $\hat{\rho}$ represents a pure ensemble, the so does the projected state operator.

In general, filters can be represented mathematically by the application of projection operators onto the state operator as above.
The von Neumann Equation

We now re-derive the equation of motion for the state operator. The Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi_i\rangle = \hat{H}|\psi_i\rangle \to -i\hbar\frac{\partial}{\partial t}\langle\psi_i| = \langle\psi_i|\hat{H}$$
(15.216)

gives

$$\begin{aligned} \frac{\partial \hat{\rho}}{\partial t} &= \frac{\partial}{\partial t} \left[\sum_{i} p_{i} \left| \psi_{i} \right\rangle \left\langle \psi_{i} \right| \right] = \sum_{i} p_{i} \left(\left(\frac{\partial}{\partial t} \left| \psi_{i} \right\rangle \right) \left\langle \psi_{i} \right| + \left| \psi_{i} \right\rangle \left(\frac{\partial}{\partial t} \left\langle \psi_{i} \right| \right) \right) \\ &= \frac{1}{i\hbar} \sum_{i} p_{i} \left(\hat{H} \left| \psi_{i} \right\rangle \left\langle \psi_{i} \right| - \left| \psi_{i} \right\rangle \left\langle \psi_{i} \right| \hat{H} \right) = \frac{1}{i\hbar} \left[\hat{H}, \sum_{i} p_{i} \left| \psi_{i} \right\rangle \left\langle \psi_{i} \right| \right] \\ &= -\frac{i}{\hbar} \left[\hat{H}, \hat{\rho} \right] \end{aligned}$$
(15.217)

which is the *von Neumann equation*. This holds for time-dependent Hamiltonians also. It describes the time evolution of the state operator in the Schrodinger picture.

Now, if we start in the state $|\psi(t_0)\rangle$ at time t_0 , then we have the formal solution of the Schrödinger equation

$$|\psi(t)\rangle = \hat{U}(t,t_0) |\psi(t_0)\rangle$$
 (15.218)

where

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0)$$
(15.219)

We then get

$$\begin{split} \frac{\partial \hat{\rho}(t)}{\partial t} &= -\frac{i}{\hbar} \left[\hat{H}, \hat{\rho} \right] = -\frac{i}{\hbar} \left[\hat{H}, \sum_{i} p_{i} \left| \psi_{i} \right\rangle \left\langle \psi_{i} \right| \right] \\ &= -\frac{i}{\hbar} \left[\hat{H}, \sum_{i} p_{i} \hat{U}(t, t_{0}) \left| \psi(t_{0}) \right\rangle \left\langle \psi(t_{0}) \right| \hat{U}^{+}(t, t_{0}) \right] \\ &= -\frac{i}{\hbar} \sum_{i} p_{i} \hat{H} \hat{U}(t, t_{0}) \left| \psi(t_{0}) \right\rangle \left\langle \psi(t_{0}) \right| \hat{U}^{+}(t, t_{0}) \\ &\quad + \frac{i}{\hbar} \sum_{i} p_{i} \hat{U}(t, t_{0}) \left| \psi(t_{0}) \right\rangle \left\langle \psi(t_{0}) \right| \hat{U}^{+}(t, t_{0}) \hat{H} \\ &= \sum_{i} p_{i} \frac{\partial}{\partial t} \hat{U}(t, t_{0}) \left| \psi(t_{0}) \right\rangle \left\langle \psi(t_{0}) \right| \hat{U}^{+}(t, t_{0}) \\ &\quad + \sum_{i} p_{i} \hat{U}(t, t_{0}) \left| \psi(t_{0}) \right\rangle \left\langle \psi(t_{0}) \right| \frac{\partial}{\partial t} \hat{U}^{+}(t, t_{0}) \\ &= \frac{\partial}{\partial t} \left(\hat{U}(t, t_{0}) \left| \psi(t_{0}) \right\rangle \left\langle \psi(t_{0}) \right| \hat{U}^{+}(t, t_{0}) \right) \\ &= \frac{\partial}{\partial t} \left(\hat{U}(t, t_{0}) \hat{\rho}(t_{0}) \hat{U}^{+}(t, t_{0}) \right) \end{split}$$

$$\hat{\rho}(t) = \hat{U}(t, t_0)\hat{\rho}(t_0)\hat{U}^+(t, t_0)$$
(15.220)

Theorem: The quantity $Tr\hat{\rho}^2$ is time independent. Hence, a pure(mixed) state remains a pure(mixed) state.

Proof:

$$Tr\hat{\rho}^{2}(t) = Tr\hat{U}\hat{\rho}(t_{0})\hat{U}^{+}\hat{U}\hat{\rho}(t_{0})\hat{U}^{+} = Tr\hat{U}\hat{\rho}(t_{0})\hat{I}\hat{\rho}(t_{0})\hat{U}^{+}$$
$$= Tr\hat{U}\hat{\rho}(t_{0})\hat{\rho}(t_{0})\hat{U}^{+} = Tr\hat{\rho}(t_{0})\hat{\rho}(t_{0})\hat{U}^{+}\hat{U} = Tr\hat{\rho}^{2}(t_{0})$$

Therefore, if $Tr\hat{\rho}^2(t_0) = 1$, then $Tr\hat{\rho}^2(t) = 1$ and the state remains pure and similarly for the mixed state. The expectation value in the two pictures is given by

$$\left\langle \hat{A} \right\rangle = Tr\left(\hat{\rho}(t)\hat{A}\right) = Tr\left(\hat{\rho}(t_0)\hat{A}_H(t)\right)$$
(15.221)

or the time dependence comes from the state operator in the Schrödinger picture and from the operator in the Heisenberg picture.

Spin = 1/2 **Systems**

How things actually work is particularly transparent in state spaces of *low dimension*. We consider spin = 1/2 (a 2-dimensional state space). The states (in Dirac and spinor notation)

$$|\uparrow\rangle \to \chi_{+} = \begin{pmatrix} 1\\0 \end{pmatrix} \text{ and } |\downarrow\rangle \to \chi_{-} = \begin{pmatrix} 0\\1 \end{pmatrix}$$
 (15.222)

are eigenstates of $\hat{\sigma}_z$, i.e., $\hat{\sigma}_z \chi_{\pm} = \pm \chi_{\pm}$. Now a rotation in spin space through an angle θ about an axis \hat{n} is represented by the unitary operator

$$\hat{U} = e^{\frac{i}{2}\theta\hat{n}\cdot\hat{\sigma}} = \cos\frac{\theta}{2}\hat{I} + i\hat{n}\cdot\hat{\sigma}\sin\frac{\theta}{2}$$
(15.223)

and

$$e^{\frac{i}{2}\theta\hat{n}\cdot\hat{\sigma}}\hat{m}\cdot\hat{\sigma}e^{-\frac{i}{2}\theta\hat{n}\cdot\hat{\sigma}} = \left(\cos\frac{\theta}{2}\hat{I} + i\hat{n}\cdot\hat{\sigma}\sin\frac{\theta}{2}\right)(\hat{m}\cdot\hat{\sigma})\left(\cos\frac{\theta}{2}\hat{I} - i\hat{n}\cdot\hat{\sigma}\sin\frac{\theta}{2}\right)$$
$$= \cos^{2}\frac{\theta}{2}(\hat{m}\cdot\hat{\sigma}) + i\left[\hat{n}\cdot\hat{\sigma},\hat{m}\cdot\hat{\sigma}\right]\sin\frac{\theta}{2}\cos\frac{\theta}{2} + (\hat{n}\cdot\hat{\sigma})(\hat{m}\cdot\hat{\sigma})(\hat{n}\cdot\hat{\sigma})\sin^{2}\frac{\theta}{2}$$

Now

$$(\hat{n}\cdot\hat{\sigma})(\hat{m}\cdot\hat{\sigma}) = \hat{n}\cdot\hat{m}\hat{I} + i\hat{\sigma}\cdot(\hat{n}\times\hat{m})$$
(15.224)

 or

$$[(\hat{n}\cdot\hat{\sigma}),(\hat{m}\cdot\hat{\sigma})] = 2i\hat{\sigma}\cdot(\hat{n}\times\hat{m})$$
(15.225)

Alternatively,

$$[(\hat{n}\cdot\hat{\sigma}),(\hat{m}\cdot\hat{\sigma})] = n_i m_j [\hat{\sigma}_i,\hat{\sigma}_j] = 2i\varepsilon_{ijk}n_i m_j\hat{\sigma}_k = 2i\varepsilon_{kij}n_i m_j\hat{\sigma}_k$$
$$= 2i\hat{\sigma}_k (\hat{n}\times\hat{m})_k = 2i\hat{\sigma}\cdot(\hat{n}\times\hat{m}) = -2i\hat{m}\cdot(\hat{n}\times\hat{\sigma}) \qquad (15.226)$$

or

Therefore,

$$e^{\frac{i}{2}\theta\hat{n}\cdot\hat{\sigma}}\hat{m}\cdot\hat{\sigma}e^{-\frac{i}{2}\theta\hat{n}\cdot\hat{\sigma}} = \cos^{2}\frac{\theta}{2}(\hat{m}\cdot\hat{\sigma}) + i\left[2i\hat{\sigma}\cdot(\hat{n}\times\hat{m})\right]\sin\frac{\theta}{2}\cos\frac{\theta}{2}$$

$$+ (\hat{n}\cdot\hat{\sigma})(\hat{n}\cdot\hat{m} + i\hat{\sigma}\cdot(\hat{n}\times\hat{m}))\sin^{2}\frac{\theta}{2}$$

$$= (\hat{m}\cdot\hat{n})(\hat{n}\cdot\hat{\sigma})\sin^{2}\frac{\theta}{2} + (\hat{m}\cdot(\hat{n}\times\hat{\sigma}))\sin\theta + (\hat{m}\cdot\hat{\sigma})\cos^{2}\frac{\theta}{2}$$

$$+ i(\hat{n}\cdot\hat{\sigma})((\hat{n}\times\hat{m})\cdot\hat{\sigma})\sin^{2}\frac{\theta}{2}$$

$$= (\hat{m}\cdot\hat{n})(\hat{n}\cdot\hat{\sigma})\sin^{2}\frac{\theta}{2} + (\hat{m}\cdot(\hat{n}\times\hat{\sigma}))\sin\theta + (\hat{m}\cdot\hat{\sigma})\cos^{2}\frac{\theta}{2}$$

$$+ i(\hat{n}\cdot(\hat{n}\times\hat{m}) + i\hat{\sigma}\cdot(\hat{n}\times(\hat{n}\times\hat{m}))\sin^{2}\frac{\theta}{2}$$

$$= (\hat{m}\cdot\hat{n})(\hat{n}\cdot\hat{\sigma})\sin^{2}\frac{\theta}{2} + (\hat{m}\cdot(\hat{n}\times\hat{\sigma}))\sin\theta + (\hat{m}\cdot\hat{\sigma})\cos^{2}\frac{\theta}{2}$$

$$- (\hat{n}\times\hat{m})\cdot(\hat{n}\times\hat{\sigma})\sin^{2}\frac{\theta}{2}$$

$$= (\hat{m}\cdot\hat{n})(\hat{n}\cdot\hat{\sigma})\sin^{2}\frac{\theta}{2} + (\hat{m}\cdot(\hat{n}\times\hat{\sigma}))\sin\theta + (\hat{m}\cdot\hat{\sigma})\cos^{2}\frac{\theta}{2}$$

$$- (\hat{m}\cdot\hat{\sigma} - (\hat{m}\cdot\hat{n})(\hat{n}\cdot\hat{\sigma}))\sin^{2}\frac{\theta}{2}$$

$$= (\hat{m}\cdot\hat{n})(\hat{n}\cdot\hat{\sigma})\sin^{2}\frac{\theta}{2} + (\hat{m}\cdot(\hat{n}\times\hat{\sigma}))\sin\theta - ((\hat{m}\cdot(\hat{n}\times(\hat{n}\times\hat{\sigma})))$$

$$+ (\hat{m}\cdot\hat{n})(\hat{n}\cdot\hat{\sigma}))\cos^{2}\frac{\theta}{2} + (\hat{m}\cdot(\hat{n}\times\hat{\sigma}))\cos\theta + (\hat{m}\cdot(\hat{n}\times\hat{\sigma}))\sin\theta$$

$$(15.227)$$

or

$$e^{\frac{i}{2}\theta\hat{n}\cdot\hat{\sigma}}\hat{\sigma}e^{-\frac{i}{2}\theta\hat{n}\cdot\hat{\sigma}} = \hat{n}\left(\hat{n}\cdot\hat{\sigma}\right) - \left(\hat{n}\times(\hat{n}\times\hat{\sigma})\right)\cos\theta + \left(\hat{n}\times\hat{\sigma}\right)\sin\theta \qquad (15.228)$$

For rotations about the $x-{\rm axis}$ these reduce to (using \hat{n} = $\hat{x})$

$$\hat{U}_x = e^{\frac{i}{2}\theta\sigma_x} = \cos\frac{\theta}{2}\hat{I} + i\sigma_x\sin\frac{\theta}{2} = \cos\frac{\theta}{2}\hat{I} + i\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\sin\frac{\theta}{2}$$
(15.229)

$$e^{\frac{i}{2}\theta\sigma_{x}}\hat{t}\cdot\hat{\sigma}e^{-\frac{i}{2}\theta\sigma_{x}} = (\hat{t}\cdot\hat{x})(\hat{x}\cdot\hat{\sigma}) - \hat{t}\cdot(\hat{x}\times(\hat{x}\times\hat{\sigma}))\cos\theta + \hat{t}\cdot(\hat{x}\times\hat{\sigma})\sin\theta$$

$$= t_{x}\sigma_{x} - \hat{t}\cdot(\hat{x}\times(\sigma_{y}\hat{z}-\sigma_{z}\hat{y}))\cos\theta + \hat{t}\cdot(\sigma_{y}\hat{z}-\sigma_{z}\hat{y})\sin\theta$$

$$= t_{x}\sigma_{x} - \hat{t}\cdot(-\sigma_{y}\hat{y}-\sigma_{z}\hat{z})\cos\theta + \hat{t}\cdot(\sigma_{y}\hat{z}-\sigma_{z}\hat{y})\sin\theta$$

$$= t_{x}\sigma_{x} + (\sigma_{y}t_{y}+\sigma_{z}t_{z})\cos\theta + (\sigma_{y}t_{z}-\sigma_{z}t_{y})\sin\theta$$

$$= (t_{x},t_{y},t_{z})\begin{pmatrix} 1 & 0 & 0\\ 0 & \cos\theta & -\sin\theta\\ 0 & \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \sigma_{x}\\ \sigma_{y}\\ \sigma_{z} \end{pmatrix}$$
(15.230)

The eigenstates of $\hat{t} \cdot \hat{\sigma}$, i.e., the eigenstates of spin = 1/2 in the \hat{t} direction are given by the equation

$$\hat{U}_x(\hat{t}\cdot\hat{\sigma})\hat{U}_x^+\chi_{\pm} = e^{\frac{i}{2}\theta\sigma_x}(\hat{t}\cdot\hat{\sigma})e^{-\frac{i}{2}\theta\sigma_x}\chi_{\pm} = \pm\chi_{\pm}$$
(15.231)

 or

$$(\hat{t} \cdot \hat{\sigma})(\hat{U}_x^+ \chi_{\pm}) = \pm (\hat{U}_x^+ \chi_{\pm})$$
 (15.232)

The two eigenfunctions are

$$\hat{U}_{x}^{+}\chi_{+} = \begin{pmatrix} \cos\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} \end{pmatrix} , \quad \hat{U}_{x}^{+}\chi_{-} = \begin{pmatrix} -i\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}$$
(15.233)

Some Special Cases

For $\theta = -\pi/2$, we get the eigenfunctions of σ_y :

$$\chi_{+}^{y} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\i \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\chi_{+} + i\chi_{-}\right) \quad , \quad \chi_{-}^{y} = \frac{1}{\sqrt{2}} \begin{pmatrix} i\\1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(i\chi_{+} + \chi_{-}\right)$$
(15.234)

and similarly for the eigenfunctions of σ_x :

$$\chi_{+}^{x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\chi_{+} + \chi_{-}\right) \quad , \quad \chi_{-}^{x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\chi_{+} - \chi_{-}\right)$$
(15.235)

A rotation through 2π gives $\hat{U} = -1$ and $\chi \to -\chi$. In a rotation through 360° the spinor changes its sign. It takes a rotation through 4π to produce $\hat{U} = +1$ and $\chi \to +\chi$. This property is related to the spinor nature of χ and the transformation relation for $\hat{t} \cdot \hat{\sigma}$ is related to the vector nature of $\hat{\sigma}$.

Let us now discuss the spin part of the density matrix. Imagine we are dealing with electron beams. An electron beam of spin \uparrow has the density operator

$$\rho_{\uparrow} = |\uparrow\rangle \left\langle\uparrow\right| \tag{15.236}$$

while an electron beam of spin \downarrow has the density operator

$$\rho_{\downarrow} = \left|\downarrow\right\rangle \left\langle\downarrow\right| \tag{15.237}$$

If one mixes the two beams in a 50:50 ratio, the density operator is

$$\rho_M = \frac{1}{2} \left(\left| \uparrow \right\rangle \left\langle \uparrow \right| + \left| \downarrow \right\rangle \left\langle \downarrow \right| \right) \tag{15.238}$$

This state has unknown relative phases.

It is not a pure state since

$$\rho_M^2 = \frac{1}{2} \rho_M \neq \rho_M \tag{15.239}$$

In contrast, the pure state (a superposition instead of a mixture) has known relative phases, i.e.

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle + e^{i\alpha} |\downarrow\rangle\right) \tag{15.240}$$

and has the density operator

$$\rho_{\alpha} = \frac{1}{2} \left(|\uparrow\rangle \langle\uparrow| + |\downarrow\rangle \langle\downarrow| + e^{-i\alpha} |\uparrow\rangle \langle\uparrow| + e^{i\alpha} |\downarrow\rangle \langle\downarrow| \right)$$
(15.241)

In the pure state case, we clearly have *interference terms*. We can also see the differences in the matrix representations, which are given by

$$\rho_{nm} = \langle n | \rho | m \rangle \tag{15.242}$$

In these two cases we get

$$\rho_M = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad \rho_\alpha = \frac{1}{2} \begin{pmatrix} 1 & e^{-i\alpha} \\ e^{i\alpha} & 1 \end{pmatrix}$$
(15.243)

The mixed state density operator is diagonal.

The difference between the two density operators shows up in expectation values and hence has measurable consequences. For the pure state,

$$\begin{split} \left\langle \hat{A} \right\rangle_{\alpha} &= Tr\left(\rho_{\alpha}\hat{A}\right) = Tr\left(\frac{1}{2} \left(\begin{array}{cc} 1 & e^{-i\alpha} \\ e^{i\alpha} & 1 \end{array}\right) \left(\begin{array}{cc} \left\langle 1|\hat{A}|1 \right\rangle & \left\langle 1|\hat{A}|2 \right\rangle \\ \left\langle 2|\hat{A}|1 \right\rangle & \left\langle 2|\hat{A}|2 \right\rangle \end{array}\right) \right) \\ &= \frac{1}{2}Tr\left(\begin{array}{cc} \left\langle 1|\hat{A}|1 \right\rangle + e^{-i\alpha} \left\langle 2|\hat{A}|1 \right\rangle & \left\langle 1|\hat{A}|2 \right\rangle + e^{-i\alpha} \left\langle 2|\hat{A}|2 \right\rangle \\ e^{i\alpha} \left\langle 1|\hat{A}|1 \right\rangle + \left\langle 2|\hat{A}|1 \right\rangle & e^{i\alpha} \left\langle 1|\hat{A}|2 \right\rangle + \left\langle 2|\hat{A}|2 \right\rangle \end{array}\right) \\ &= \frac{1}{2}\left(\left\langle 1|\hat{A}|1 \right\rangle + \left\langle 2|\hat{A}|2 \right\rangle + 2\operatorname{Re}\left(e^{i\alpha} \left\langle 1|\hat{A}|2 \right\rangle\right)\right) \end{split}$$

while for the mixed state we have

$$\begin{split} \left\langle \hat{A} \right\rangle_{M} &= Tr\left(\rho_{M}\hat{A}\right) = Tr\left(\frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \langle 1|\hat{A}|1\rangle & \langle 1|\hat{A}|2\rangle \\ \langle 2|\hat{A}|1\rangle & \langle 2|\hat{A}|2\rangle \end{pmatrix} \right) \\ &= \frac{1}{2}Tr\left(\begin{array}{c} \langle 1|\hat{A}|1\rangle & \langle 1|\hat{A}|2\rangle \\ \langle 2|\hat{A}|1\rangle & \langle 2|\hat{A}|2\rangle \end{pmatrix} \\ &= \frac{1}{2}\left(\langle 1|\hat{A}|1\rangle + \langle 2|\hat{A}|2\rangle \right) \end{split}$$

Again, we see no interference (quantum) effects from the mixed state. It is clear from these expressions that the mixed-state expectation value arises from the pure-state expectation value by *averaging over the relative phase value*, i.e.,

$$\rho_M = \frac{1}{2\pi} \int_0^{2\pi} \rho_\alpha d\alpha \tag{15.244}$$

Polarization of Spin = 1/2 **Particles**

The most general density operator in spin space is given by

$$\hat{\rho} = \frac{1}{2} \left(\hat{I} + \vec{b} \cdot \vec{\sigma} \right) \tag{15.245}$$

since the set of four matrices $\hat{I}, \hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3$ is a basis for all 2×2 matrices. The property $Tr\hat{\rho} = 1$ works because $Tr\hat{I} = 2$ and $Tr\hat{\sigma}_i = 0$. If we choose \vec{b} to point in the z-direction, then we have

$$\hat{\rho} = \frac{1}{2} \left(\hat{I} + b\hat{\sigma}_z \right) = \frac{1}{2} \left(\begin{array}{cc} 1+b & 0\\ 0 & 1-b \end{array} \right)$$
(15.246)

This implies that $(1 \pm b)/2$ are probabilities and thus we must have $|\vec{b}| \leq 1$. If we have a pure state, then we must also have $\hat{\rho}^2 = \hat{\rho}$, which implies that

$$\hat{\rho}^2 = \frac{1}{4} \left(\hat{I} + 2\vec{b} \cdot \vec{\sigma} + (\vec{b} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) \right) = \frac{1}{4} \left(\hat{I} + 2\vec{b} \cdot \vec{\sigma} + b^2 \hat{I} \right)$$
$$= \frac{1}{2} \left(\frac{1 + b^2}{2} \hat{I} + \vec{b} \cdot \vec{\sigma} \right) = \hat{\rho} = \frac{1}{2} \left(\hat{I} + \vec{b} \cdot \vec{\sigma} \right) \hat{\rho}^2 = \hat{\rho}$$

or $|\vec{b}| = 1$ in the pure state case. Now a straightforward calculation gives

$$\begin{split} \langle \hat{\sigma}_i \rangle &= Tr \hat{\rho} \hat{\sigma}_i = Tr \left[\frac{1}{2} \left(\hat{I} + \vec{b} \cdot \vec{\sigma} \right) \hat{\sigma}_i \right] \\ &= Tr \left[\frac{1}{2} \hat{\sigma}_i \right] + Tr \left[\frac{1}{2} (\vec{b} \cdot \vec{\sigma}) \hat{\sigma}_i \right] = Tr \left[\frac{1}{2} b_i \hat{I} \right] = b_i \end{split}$$

This implies that the degree of polarization of the spin state is characterized by $b = |\vec{b}|$. The case b = 0 represents a completely polarized beam.

(4) The Measurement Process

We have a beams of atoms or electrons moving through the inhomogeneous field of a magnet as shown in Figure 15.8 below.

The force is given by

$$m_z \frac{\partial B_z}{\partial z} \tag{15.247}$$

which splits the beams into many beams each with a different value of m_z . We assume that the total angular momentum is spin only and S = 1/2. The motion in the *y*-direction is force-free and can be separated out. We then have the Hamiltonian

$$\hat{H} = \frac{\hat{p}_z^2}{2m} + B(z)\mu_B\hat{\sigma}_z \approx \frac{\hat{p}_z^2}{2m} + (B + B'z +)\mu_B\hat{\sigma}_z$$
(15.248)



Figure 15.8: Stern-Gerlach Setup

describing the motion in the z-direction. We have Taylor expanded the magnetic field. The time-development of the state vector is given by the equation

$$i\hbar\frac{\partial\psi}{\partial t} = i\hbar\frac{\partial}{\partial t} \begin{pmatrix} u_+\\ u_- \end{pmatrix} = \hat{H}\psi = \hat{H} \begin{pmatrix} u_+\\ u_- \end{pmatrix}$$
(15.249)

$$i\hbar\frac{\partial u_{\pm}}{\partial t} = \left(\frac{\hat{p}_z^2}{2m} \pm B\mu_B \pm B'\mu_B z\right)u_{\pm}$$
(15.250)

If we let the spatial wavefunction be a wave packet f(z) concentrated about the z-axis before entering the magnetic field at time t = 0, then at time t, it is then approximately

$$u_{\pm}(z,t) = f(z \pm Ct^2)e^{\mp i\alpha t}$$
 (15.251)

where the constant

$$C = \frac{B'\mu_B}{2m} \tag{15.252}$$

is the acceleration during the period the particle is in the magnetic field region and

$$\alpha = \frac{B\mu_B}{\hbar} \tag{15.253}$$

This says that the particles with spin \uparrow and \downarrow are deflected downwards and upwards, respectively.

The Stern-Gerlach Experiment as a Model for an Idealized Measurement

In this experiment the object being measured is the spin of the particle and the measuring apparatus is the position of the particle after traversing the magnetic field (location on some screen). After passing through the magnetic field we know that

for
$$\uparrow$$
, $z < 0$ and for \downarrow , $z > 0$ (15.254)

This apparatus, whose readout (position of some pointer) is the z-coordinate of the particle, is thus appropriate for distinguishing \uparrow from \downarrow and, by the actual

size of the deflection, for determining the size of the magnetic moment and hence the spin.

The requirement that the z-coordinate of the particle serve as the pointer of a measuring instrument implies that the deflections must be macroscopically distinguishable. Formally, this implies that the overlap of the two wave packets $f(z + Ct^2)$ and $f(z - Ct^2)$ must be negligible. We also assume that we have calibrated the device.

What happens to general states?

We consider the initial state(a superposition)

$$\psi(z,0) = \frac{1}{\sqrt{2}} \left(\chi_+ + \chi_- \right) f(z) \tag{15.255}$$

After traversing the field this becomes

$$\psi(z,t) = \frac{1}{\sqrt{2}} \left(\chi_+ f(z+Ct^2) e^{-i\alpha t} + \chi_- f(z-Ct^2) e^{i\alpha t} \right)$$
(15.256)

The polarization and the pointer (z-coordinate) are coupled or entangled.

There is a unique correlation between the state of the spin and the state of the pointer. Neither the spin nor the pointer are in an eigenstate (neither have definite values).

In the basis of the states $|z\rangle |\pm\rangle$, the density operator is

$$\rho_{zz'} = \langle \pm | \langle z | (|\psi(t)) \langle \psi(t) |) | z' \rangle | \pm' \rangle$$

= $\frac{1}{2} \begin{pmatrix} f(z + Ct^2) f(z' + Ct^2)^* & f(z + Ct^2) f(z' - Ct^2)^* e^{-2i\alpha t} \\ f(z - Ct^2) f(z' + Ct^2)^* e^{2i\alpha t} & f(z - Ct^2) f(z' - Ct^2)^* \end{pmatrix}$
(15.257)

Measurement of spin observables

After the spin 1/2 particle has passed through the Stern-Gerlach apparatus, suppose that its spin is measured. The measurement can take place in two ways:

- (i) ignoring the pointer position z
- (ii) for a particular pointer position z

In case (i), if one ignores the pointer position, then ρ is equivalent to

$$\hat{\rho} = \int dz \left\langle z | \rho | z \right\rangle = \frac{1}{2} \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right)$$
(15.258)

This result holds because there is no overlap of the pointer wave functions $f(z + Ct^2)$ and $f(z - Ct^2)$. For an observable $F(\vec{\sigma})$, depending only on spin operators, we then have

$$Tr_{z,\sigma}\left(\rho F(\vec{\sigma})\right) = Tr_{\sigma}\left(\hat{\rho}F(\vec{\sigma})\right) \tag{15.259}$$

where the density operator $\hat{\rho}$ corresponds to a mixed ensemble. Thus, the *pure* ensemble ρ is replaced by the mixed ensemble $\hat{\rho}$.

In case (ii), filtering out the pointer position: in this case, we consider only the particles with pointer position z-positive, i.e., we construct

$$Tr_{z>0,\sigma}(\rho F(\vec{\sigma})) = \int ds \rho_{zz} = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$
(15.260)

Because of normalization, the density is operator is actually

$$\left(\begin{array}{cc} 0 & 0\\ 0 & 1 \end{array}\right) = \rho_{\downarrow} \tag{15.261}$$

The particles deflected up have the spin wave function $|\downarrow\rangle$.

For a measurement with the result z-positive(spin negative), the state goes over to $|\downarrow\rangle$. This is consistent with the quantum mechanical postulate that measurements are repeatable.

The fact that the particles which have been filtered off at a particular pointer position are in that eigenstate corresponding to the eigenvalue measured is called the *collapse or reduction* of the state vector.

Going over from ρ to $\hat{\rho}$ with respect to all observables related to spin can also be regarded as a reduction of the state vector.

The density matrix $\hat{\rho}$ describes an ensemble composed of 50% spin-up and 50% spin-down states. If N particles are subjected to this Stern-Gerlach experiment, then as far as their spins are concerned, they are completely equivalent to N/2 particles in the state $|\uparrow\rangle$ and N/2 in the state $|\downarrow\rangle$.

15.2.8 A General Experiment and Coupling to the Environment

We now consider a general experiment. Let O be the object and A the apparatus including the readout. At the time t = 0, let the state of the whole system O + A be

$$|\psi(0)\rangle = \sum_{n} c_n |O, n\rangle |A\rangle \tag{15.262}$$

where the $|O, n\rangle$ are object states and $|A\rangle$ is the (metastable) initial state of the apparatus. At a later time t, after the interaction of the object with the measuring apparatus, the state becomes

$$|\psi(t)\rangle = \sum_{n} c_n |O, n\rangle |A(n)\rangle$$
(15.263)

where the final states of the apparatus $|A(n)\rangle$. n = 1, 2, 3, must be macroscopically distinguishable.

As before the density operator for this pure states is

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| \qquad (15.264)$$

If we read off the result of the measurement, the density operator for observables relevant to the object O is

$$\hat{\rho} = Tr_{A(n)}\rho(t) = \sum_{n} |c_{n}|^{2} |O, n\rangle \langle O, n|$$
(15.265)

We needed to make use of the fact that the final states of the apparatus are macroscopically distinguishable, and thus do not overlap, i.e., that $\langle A(n) | A(m) \rangle = \delta_{mn}$.

Thus, if we do not read off the result of the measurement, a mixture occurs with respect to O. If, on the other hand, we read off a particular value, e.g., A(m), the density operator is then

$$|O,m\rangle\langle O,m| \tag{15.266}$$

The probability of measuring the value A(m) is clearly $|c_m|^2$. The fact that in a measurement with the result A(m) the density operator changes from

$$|\psi(t)\rangle\langle\psi(t)| \to |O,m\rangle\langle O,m| \tag{15.267}$$

is known as the reduction of the wave function or state vector.

We now take into account the fact that the object and the apparatus are never completely isolated from the environment, and take Z to be an additional variable representing all further macroscopic consequences which couple to the state A of the apparatus. The initial state is then

$$|\psi(0)\rangle = \sum_{n} c_n |O, n\rangle |A\rangle |Z\rangle \qquad (15.268)$$

and after passage through the apparatus the state evolves into

$$|\psi(t)\rangle = \sum_{n} c_n |O, n\rangle |A(n)\rangle |Z(n)\rangle$$
(15.269)

If we do not read off Z, which always happens in practice, since we cannot keep track of all the macroscopic consequences, the density operator of the (object + apparatus) is the mixture

$$\hat{\hat{\rho}} = \sum_{n} |c_n|^2 |A(n)\rangle |O, n\rangle \langle O, n| \langle A(n)|$$
(15.270)

The subsystem (object + apparatus) is thus a mixed state. N such subsystems behave like

$$N |c_1|^2$$
 subsystems in the state $|O, 1\rangle |A(1)\rangle$
 $N |c_2|^2$ subsystems in the state $|O, 2\rangle |A(2)\rangle$
..... $N |c_n|^2$ subsystems in the state $|O, n\rangle |A(n)\rangle$

This is a completely different density operator than that of the pure state, i.e., $|\psi(t)\rangle\langle\psi(t)|$.

(i) If we do not read off A(n) either, then $\hat{\rho}$ is equivalent to

$$\hat{\rho} = \sum_{n} \left| c_n \right|^2 \left| O, n \right\rangle \left\langle O, n \right| \tag{15.271}$$

(ii) If we read off A(n), then the probability of obtaining the particular reading A(m) is

$$Tr_{O,A}\left(|A(m)\rangle\langle A(m)|\hat{\rho}\rangle = |c_m|^2 \tag{15.272}$$

and in this case, the density operator is then

$$|A(m)\rangle|O,m\rangle\langle O,m|\langle A(m)|$$
(15.273)

From that point onwards, it does not matter if we disregard A. Taking the trace over A(n) yields, for the observable O, the density operator

$$|O,m\rangle\langle O,m| \tag{15.274}$$

The key problem in the theory of measurement is this reduction of the wave function and in particular the question of when it takes place. This problem is illustrated quite drastically by phenomena of **Schrodinger's Cat** discussed in Chapter 14.

Influence of an Observation on Time Evolution

In order to further analyze the measurement process and its impact, we return to the Stern-Gerlach experiment and consider this additional setup.

After the atomic beams have traversed the Stern-Gerlach apparatus, we recombine them by means of a complicated field configuration in such a way that all of the deformation and spreading of the wave function is carefully undone, i.e., the state

$$f(z)\left(c_1 e^{i\phi_+}\chi_+ + c_2 e^{i\phi_-}\chi_-\right) \tag{15.275}$$

is formed. This is the initial wave function once again, essentially. The phase factors are inserted to characterize any path length differences.

Now, in the region where the beams + and – are macroscopically separated, we can set up a real measuring device whose pointer Z which reacts to z by the interaction U(z-Z), so that positive (negative) z leads to positive(negative) Z. We then have for the initial state

$$|\psi_a\rangle = f(z) (c_1 \chi_+ + c_2 \chi_-) |Z = 0\rangle$$
 (15.276)

for the intermediate state

$$|\psi_c\rangle = c_1 \chi_+ f(z + Ct^2) | Z = -1 \rangle + c_2 \chi_- f(z - Ct^2) | Z = +1 \rangle$$
(15.277)

and for the state after traversing the entire setup

$$|\psi_e\rangle = f(z)(c_1\chi_+e^{i\phi_+}|Z=-1) + c_2\chi_-e^{-i\phi_+}|Z=+1\rangle)$$
(15.278)

The pointer positions are described by $|Z = 0\rangle$ and $|Z = \pm 1\rangle$.

We now compare these two situations:

I. We turn on the coupling to the measuring device ${\cal Z}$ and obtain the final state

$$|\psi_e\rangle = f(z)(c_1\chi_+e^{i\phi_+}|Z=-1) + c_2\chi_-e^{-i\phi_+}|Z=+1\rangle)$$
(15.279)

II. We turn off the coupling to the measuring device Z and obtain the final state

$$|\psi_e\rangle = f(z) \left(c_1 e^{i\phi_+} \chi_+ + c_2 e^{i\phi_-} \chi_- \right) | Z = 0 \right)$$
(15.280)

The resulting density operators are quite different. Although the state

$$|\psi_e\rangle = f(z)(c_1\chi_+e^{i\phi_+}|Z=-1) + c_2\chi_-e^{-i\phi_+}|Z=+1\rangle)$$
(15.281)

is a pure state, it is equivalent to a mixture, as far as the statements relating to the particle are concerned. This is due to the fact that the macroscopic states $|Z = \pm 1\rangle$ do not overlap (they are orthogonal).

In situation II, both the total state and the state of the atom are pure states, In situation I, the final state of the total system (atom + pointer) (characterized by spin z and Z), is mixed, unless c_1 or c_2 vanish.

Evidently, the physical situation differs according to whether the interaction U(z-Z) between the system and the pointer is turned on or not.

Even if we do not read the result, we still influence the atomic system.

In order to further illustrate the back-reaction of the experiment on the object, we now consider the following thought experiment due to Heisenberg. We connect two Stern-Gerlach devices in series as shown in Figure 15.9 below



Figure 15.9: Back Reaction Experiment

Let the initial state of the atoms in the atomic beam be $|a\rangle$, let $\{|e\rangle\}$ be a basis for the final states, and let $\{|c\rangle\}$ be a basis for the intermediate state. We now determine the probability of transition to the final state $|e\rangle$, by representing this in terms of the transition amplitudes of $|a\rangle$ to $|c\rangle$ to $|e\rangle$.

For an isolated system the transition probability is

$$P_{a \to e}^{I} = \left| \sum_{c} U_{ac}^{(1)} U_{ce}^{(2)} \right|^{2}$$
(15.282)

because

$$\sum_{c} U_{ac}^{(1)} U_{ce}^{(2)} = U_{ae} \tag{15.283}$$

holds for an isolated system.

On the other hand, one could also say that the transition probability is the product of the probabilities

$$\left|U_{ac}^{(1)}\right|^{2}\left|U_{ce}^{(2)}\right|^{2} \tag{15.284}$$

summed over all intermediate states \boldsymbol{c} :

$$P_{a \to e}^{II} = \sum_{c} \left| U_{ac}^{(1)} \right|^2 \left| U_{ce}^{(2)} \right|^2 \tag{15.285}$$

These two probability expressions correspond to different experiments.

For $P_{a \to e}^{II}$ there is a measurement in the intermediate region, and this introduces unknown phase factors $e^{i\phi_c}$ which must be averaged over.

Experiment 1: Between SG_1 and SG_2 , the atoms remain unperturbed. There is no coupling to the external world, and the transition probability is $P_{a \to e}^I$.

Experiment 2: Between SG_1 and SG_2 , there is an influence on the atoms, making possible a determination of the stationary state. However, the result

of the measurement is not recorded, and a mixture is formed. The transition probability is $P^I_{a \to e} I$.

Experiment 3: Between SG_1 and SG_2 , an influence on the atoms occurs making possible a determination of the stationary state. Let us assume that c is found. The probability for state $|e\rangle$ behind SG_2 is then given by $|U_{ce}^{(2)}|^2$.

15.3 Kochen-Specker Theorem

Some, perhaps many, users of quantum theory may find a pragmatic approach (or interpretation), where a sharp distinction is made between the system and the observer or observing equipment(or even a full instrumentalist interpretation, where the primary emphasis is placed on the act of measurement with quantum theory being viewed as a scheme for predicting the probabilistic spread of the results obtained) satisfactory, but it is hard to believe that either gives the ultimate view of physical reality. Indeed, with their reluctance to grant objective status to the properties of individual systems, it is arguable whether either gives a picture of reality at all.

However, attempts to move towards a more realist philosophy by ascribing *latent* properties to individual systems most often tend to be too vague to do much more than stimulate a search for new conceptual categories. In particular, there is the unresolved issue of how the transition from potentiality to actuality is made in realistic interpretations.

It is not surprising, therefore, that many physicists have sought an interpretation of quantum theory in which the probabilistic results would have the same status as those in classical statistical physics where almost all of these difficult philosophical problems do not arise.

Most discussions of this type involve the epistemic interpretation of probability, in which probabilistic assignments refer to our knowledge of an objectively existing state of affairs, for example, an expression like $\Delta_{\psi}A$ (the dispersion) would be a measure of our ignorance of A which, it is supposed, does have an actual value. Such a position is consistent with a completely realist view of the world, in which individual objects and properties have an unequivocal existence that is independent of any act of observation or measurement.

Interpretations of this type are naturally coupled with the assumptions that

- 1. quantum states refer to individual systems directly, not just to the outcome of repeated measurements, or to any associated ensemble of systems
- 2. a (perfect) measurement of a physical quantity reveals the value that it possessed immediately beforehand

Most problems discussed by quantum theorists would not arise in a scheme where properties are possessed in this way. For example, state-vector reduction would merely be an acquisition of further knowledge about the system by making a measurement - a clear analogue of the classical idea of conditional probability. True, this raises the question of whether the measurement itself can be described in quantum-mechanical terms, but the significance of this problem, in this case, is no greater than it is in classical statistical physics.

Since an epistemic interpretation of quantum theory promises to remove most of the conceptual problems, one might wonder why the theory is not automatically presented in this way from the outset.

The reason is that the concept of an individual system *possessing* a value for all its physical quantities is difficult to reconcile with the actual formalism of quantum theory. As we have seen, one obstacle to this view are the Bell inequalities, as discussed earlier in Chapter 8 and will discuss extensively in Chapter 16.

Another obstacle is the Kochen-Specker theorem, which we discuss now. We are concerned here with the existence of a value function $V_{|\psi\rangle}(A)$ that is to be interpreted as the value of the physical quantity A when the quantum state (of an individual system) is $|\psi\rangle$. There is no difficulty with this concept in classical physics, where, to each physical quantity A there corresponds a function $f_A: S \to \Re$ (where S is the classical state space) such that the value of A in the state $s \in S$ is just the value of f_A at s:

$$V_s(A) = f_A(s)$$
 (15.286)

The situation in quantum mechanics is very different since we have no prima facie idea how to specify the value of $V_{|\psi\rangle}(A)$ for any particular pair $(A, |\psi\rangle)$. If $|\psi\rangle$ is an eigenvector $|a\rangle$ of the self-adjoint operator \hat{A} that represents A, then we might be inclined to say that $V_{|a\rangle}(A) = a$, where a is the corresponding eigenvalue, but it is unclear how to go beyond this special case.

As a consequence, nothing useful can be said about the existence of quantum value-functions without postulating further properties for them.

We note that there are plenty of functions that satisfy the eigenvector requirement. For example, the function

$$V_{|\psi\rangle}(A) = \langle \psi | \hat{A} | \psi \rangle \tag{15.287}$$

does so (assuming that $|\psi\rangle$ is normalized). However, as we know, this gives the expected value of A, so it is not a good choice for a value function in any situation in which the dispersion $\Delta_{\psi}A$ is non-zero. Therefore, to get a sensible notion of a value function it is clearly necessary to go beyond the eigenvector requirement. The most natural condition to impose is that, for any function $F: \mathfrak{R} \to \mathfrak{R}$,

$$V_{|\psi\rangle}(F(A)) = F(V_{|\psi\rangle}(A)) \qquad \text{[condition A]} \qquad (15.288)$$

Thus, in any quantum state $|\psi\rangle$, the value of a function of a physical quantity is equal to the function evaluated on the value of the quantity; for example, the value of L_x^2 is the square of the value of the angular momentum L_x .

Earlier we discussed the meaning of the expression F(A).

If we are quantizing a given classical system with state space S then F(A) can stand for $F(f_A)(s)$, where $f_A : S \to \mathfrak{R}$, and where the map $F(f_A) : S \to \mathfrak{R}$ is defined by $F(f_A)(s) := F(f_A(s))$ for all $s \in S$. In this case, it is viable to regard a value function $V_{|\psi\rangle}$ as being defined on real-valued functions f on the classical state space S.

However, if we do not wish to assume any such classical background, then something different is needed.

One possibility is to define F(A) as that physical quantity which is associated with the operator $F(\hat{A})$. Of course, this is only meaningful if the quantization map from physical quantity to self-adjoint operator is

- (1) **onto** so that $F(\hat{A})$ is the quantum representative of *some* physical quantity.
- (2) **one-to-one** so that the quantity thus defined is *unique*.

Under these circumstances, nothing is lost by thinking of $V_{|\psi\rangle}$ as a function of self-adjoint operators, rather than physical quantities.

Another way of looking at this whole argument is to start with a value-function $V'_{|\psi\rangle}$ that is a function of *self-adjoint operators*, rather than physical quantities. The analogue of the condition A above is then the relation

$$V'_{|\psi\rangle}(F(\hat{A})) = F(V'_{|\psi\rangle}(\hat{A}))$$
(15.289)

which deals only with mathematical entities. A value-function $V_{|\psi\rangle}$ of physical quantities can then be defined by

$$V_{|\psi\rangle}(A) \coloneqq V'_{|\psi\rangle}(\hat{A}) \tag{15.290}$$

If the quantization map is one-to-one and onto, then F(A) is well-defined as the inverse image of $F(\hat{A})$, and the $V_{|\psi\rangle}$ function constructed in this way satisfies condition A.

Note that we are driven towards such a strategy because, on the one hand(and unlike in the pragmatic approach), an operational definition in terms of *measurements* is not appropriate in the context of the more realist interpretation

being sought. But, on the other hand, we must avoid defining F(A) to be the physical quantity that satisfies condition A for all $|\psi\rangle \in \mathcal{H}$, since, then condition A would be a tautology. The potential trap is that this is precisely how a function of a physical quantity is defined in classical physics. This discussion impinges also on the basic function-preserving requirement $F(A) = F(\hat{A})$, which does become a tautology if F(A) is defined to be the physical quantity that is associated with the operator $F(\hat{A})$.

The intuitively plausible requirement of condition A has the following important implications (all can be proved).

1. If $[\hat{A}, \hat{B}] = 0$, the value function is additive in the sense that, for all $|\psi\rangle \in \mathcal{H}$

$$V_{|\psi\rangle}(A+B) = V_{|\psi\rangle}(A) + V_{|\psi\rangle}(B)$$
(15.291)

where A + B denotes the physical quantity associated with the self-adjoint operator $\hat{A} + \hat{B}$.

2. If $[\hat{A}, \hat{B}] = 0$, the value function is multiplicative in the sense that, for all $|\psi\rangle \in \mathcal{H}$

$$V_{|\psi\rangle}(AB) = V_{|\psi\rangle}(A)V_{|\psi\rangle}(B) \tag{15.292}$$

where AB denotes the physical quantity associated with the self-adjoint operator $\hat{A}\hat{B}$.

3. Let *I* denote the physical quantity that corresponds to the identity operator \hat{I} . Then using the result in (2) above with $A \coloneqq I$, we see that, for each state $|\psi\rangle$

$$V_{|\psi\rangle}(B) = V_{|\psi\rangle}(I)V_{|\psi\rangle}(B)$$
(15.293)

for all physical quantities B. Thus, for each $|\psi\rangle \in \mathcal{H}$, we get

$$V_{|\psi\rangle}(I) = 1 \tag{15.294}$$

provided that there is at least one quantity B for which $V_{|\psi\rangle}(B) \neq 0$.

The multiplicative property of (2) above has an important implication for any physical quantity P whose representative is a projection operator \hat{P} . In this case, the property $\hat{P}^2 = \hat{P}$ implies at once that

$$(V_{|\psi\rangle}(P))^2 = V_{|\psi\rangle}(P^2) = V_{|\psi\rangle}(P)$$
 (15.295)

and hence

$$V_{|\psi\rangle}(P) = 0 \ or \ 1 \tag{15.296}$$

Thus, thinking of P as a proposition, we see that a quantum value function $V_{|\psi\rangle}$ gives it a **false** or **true** assignment in the state $|\psi\rangle$.

Now consider a collection $\{\hat{P}_1, \hat{P}_2, \dots, \hat{P}_n\}$ of projection operators that forms a resolution of the identity, that is,

$$\hat{P}_i \hat{P}_j = 0 \text{ if } i \neq j \qquad , \qquad \hat{P}_1 + \hat{P}_2 + \dots + \hat{P}_n = \hat{I}$$
 (15.297)

For example, these could be the spectral projectors of a self-adjoint operator \hat{A} with discrete eigenvalues, so that $\hat{P}_i = \hat{P}_{A=a_i}$. In a realist interpretation, the associated proposition P_i asserts that A has a particular value a_i , which implies that the collection of propositions $\{\hat{P}_1, \hat{P}_2, \dots, \hat{P}_n\}$ should be *mutually exclusive* - only one can be true at any given time - and *exhaustive* - at least one of them must be true at any given time. This is in accord with the commonsense view of the nature of truth and falsity, that is, in a set of mutually exclusive and exhaustive propositions one and only one can be true and the rest are false. This expectation is borne out by the formalism. Indeed, the results above imply that

$$V_{|\psi\rangle}(A+B) = V_{|\psi\rangle}(A) + V_{|\psi\rangle}(B)$$
(15.298)

$$V_{|\psi\rangle}(\sum_{i=1}^{n} P_i) = \sum_{i=1}^{n} V_{|\psi\rangle}(P_i) = 1$$
(15.299)

for all states $|\psi\rangle$.

However, since each $V_{|\psi\rangle}(P_i)$ has the value 0 or 1, this sum can equal 1 only if one of the propositions is given the value 1 and the rest are given the value 0.

A special case is when $\hat{P}_i := |e_i\rangle \langle e_i|$ where $\{|e_1\rangle, |e_2\rangle, \dots$ } is an orthonormal basis for the Hilbert space \mathcal{H} . Then, according to the result just obtained above, for any state $|\psi\rangle$ a value function $V_{|\psi\rangle}$ must assign the number 1 to one of the projectors/one-dimensional subspaces (more precisely, to the associated proposition) and 0 to the rest. This is not a trivial requirement, since any given vector will belong to many different orthonormal basis sets, and the value given to the corresponding one-dimensional subspace must be independent of the choice of such a set.

In fact, this requirement is so difficult that it cannot be satisfied.

This will ultimately defeat any idea of a realist interpretation.

As stated above, this argument must apply to all possible sets of orthogonal projectors which provide a resolution of the identity in the Hilbert space. Since the projectors are in one-to-one correspondence with the rays in the Hilbert space, the above constraint means that, for every complete orthogonal basis of unit vectors in the Hilbert space, we must be able to associate the number 1 with one vector and the number 0 with all the other vectors in the basis in a consistent manner.

15.3.1 Theorem (due to Kochen and Specker)

There is no such function $V_{|\psi\rangle}$ if the

Hilbert space \mathcal{H} is such that $dim(\mathcal{H}) > 2$.

It is convenient (for carrying out a proof) to translate this problem into a coloring problem on the surface of a unit hypersphere in Hilbert space.

Translation into Coloring Problem

Can we color the hypersphere with two colors, red and blue, in such a way that the following conditions are satisfied?

- 1. Every point (unit vector) is colored red or blue.
- 2. For every complete orthogonal set of unit vectors only one is colored red.
- 3. Unit vectors belonging to the same ray have the same color.

The two-color statement of the Kochen-Specker theorem is:

If the dimension of the Hilbert space is greater than two, the coloring of the unit hypersphere in the way described above is *not* possible.

Let us denote the two-color theorem (not possible case) in a real(complex) Hilbert space of finite dimension N by $T_N^{real(complex)}$ and in an infinite-dimensional separable Hilbert space by $T_{\infty}^{real(complex)}$.

We notice at once that

$$T_N^{real} \to T_{N+1}^{real} \tag{15.300}$$

This follows by supposing the coloring is possible in the (N+1)-dimensional case (that is ~ (T_{N+1}^{real}) is true - the possible case) and considering the N-dimensional subspace orthogonal to any direction colored blue. This will now itself induce a coloring of the unit hypersphere in the subspace in accordance with the specification of the theorem. So ~ $(T_{N+1}^{real}) \rightarrow (T_N^{real})$ or contrapositively, we have proved $T_N^{real} \rightarrow T_{N+1}^{real}$.

Repeated applications of this result show that if we can prove T_N^{real} for any given N, then the theorem is true for any greater value of N and, indeed, T_{∞}^{real} will follow by a similar argument, in which, assuming the coloring is possible in the infinite-dimensional case, we show that it would be possible in a finite-dimensional subspace that includes a direction colored red.

Further, for any dimension, finite or infinite,

$$T_N^{real} \to T_N^{complex}$$
 (15.301)

since, if we could color the unit hypersphere in the Hilbert space defined over the complex field, we could show the coloring to be possible for a real Hilbert space of the same dimension by considering some particular complete orthogonal set of vectors in the complex case, and generating a structure isomorphic to a real Hilbert space by considering all the orthogonal sets obtained by real orthogonal transformations from the initial set of orthonormal vectors.

With these results in mind, all we need to do is examine T_N^{real} for low values of N. We notice that T_2^{real} is false(it is possible to satisfy conditions (1)-(3)). This corresponds to coloring the unit circle in a real Euclidean plane. The construction for doing such a coloring is shown in Figure 15.10 below.



Figure 15.10: 2-Dimensional Construction

Alternate open-closed quadrants are colored blue and red as indicated. It is then easily checked that, for any orthogonal pair of directions, one is indeed colored red and the other blue, with opposite directions having the same color.

We now show that T_3^{real} holds. First, we give a plausibility argument due to Belinfante.

Consider the unit sphere in Euclidean 3-space. Suppose that the coloring had been carried out. Then we would expect 1/3 of the surface to be colored red and 2/3 to be colored blue, since for every orthogonal triad of directions one is colored red and the remaining two blue. But every time we color a point P, say, red, then we must color the whole equator, with P as the pole, blue, since any direction orthogonal to P gets colored blue. This is shown in Figure 15.11 below.



Figure 15.11: 3-Dimensional Construction

PQR is one orthogonal triad of directions, so if P is red, then Q and R must be blue. Rotating this orthogonal triad about OP sweeps out the complete blue equator as shown. So it looks like we can never end up with enough red points,

if every red point is associated with an infinite number of blue points on the corresponding equator.

This argument , of course, is quite unrigorous, since there is a lot of double counting if one remembers that each point on a blue equator lies on infinitely many other equators!

Kochen and Specker gave a rigorous proof which goes as follows.

First, we prove a lemma:

There is a finite angular distance between any two points with opposite color.

More specifically, we shall show that if 1 and 2 are any two points on the surface of a sphere with center at O, and if we denote by θ_{12} the angle between the unit vectors $\overrightarrow{O1}$ and $\overrightarrow{O2}$, then if

$$0 \le \theta_{12} \le \sin^{-1}\left(\frac{1}{3}\right) \tag{15.302}$$

the points 1 and 2 cannot be assigned the opposite color.

Proof: We first introduce the representation of the points and orthogonality relations on the sphere by means of a so-called Kochen-Specker diagram, in which points on the sphere are represented by vertices in the diagram and if two points are in orthogonal directions, the corresponding vertices of the diagram are joined by a straight line. We show that the Kochen-Specker diagram shown in Figure 15.12 below is constructible if

$$0 \le \theta_{12} \le \sin^{-1}\left(\frac{1}{3}\right)$$

This Kochen-Specker diagram has ten points on the unit sphere in 3–dimensional Euclidean space with

$$0 \le \theta_{12} \le \sin^{-1}\left(\frac{1}{3}\right)$$

as we shall prove.

Suppose first that θ_{12} is any acute angle. Since 3 is orthogonal to 1 and 2, and 4 is orthogonal to 3, $\overrightarrow{O4}$ must be in the plane defined by $\overrightarrow{O1}$ and $\overrightarrow{O2}$. Since $\overrightarrow{O4}$ is orthogonal to $\overrightarrow{O2}$, we may choose 4 so that θ_{14} is also acute, and clearly, $\theta_{14} = \pi/2 - \theta_{12}$ as shown in Figure 15.13 below.

Now write $\overrightarrow{O5} = \hat{i}$, $\overrightarrow{O6} = \hat{k}$ and take a unit vector \hat{j} orthogonal to \hat{i} and \hat{k} so as



Figure 15.12: Kochen-Specker Diagram



Figure 15.13: Angle Diagram

to complete a set of orthonormal vectors $\{\hat{i},\hat{j},\hat{k}\}$. Then $\overrightarrow{O7}$, being orthogonal to \hat{i} , may be written as

$$\overrightarrow{O7} = (\hat{j} + x\hat{k})(1 + x^2)^{-1/2}$$
 (15.303)

Similarly,

$$\overrightarrow{O8} = (\hat{i} + y\hat{j})(1 + y^2)^{-1/2}$$
(15.304)

for some numbers x and y.

The orthogonality relations in the diagram force

$$\overrightarrow{O9} = (x\hat{j} - \hat{k})(1 + x^2)^{-1/2}$$
(15.305)

and

$$\overrightarrow{O10} = (y\hat{i} - \hat{j})(1 + y^2)^{-1/2}$$
(15.306)

But $\overrightarrow{O1}$ is orthogonal to $\overrightarrow{O7}$ and $\overrightarrow{O8}$, so we must have

$$\overrightarrow{O1} = (xy\hat{i} - x\hat{j} + \hat{k})(1 + x^2 + x^2y^2)^{-1/2}$$
(15.307)

Also, $\overrightarrow{O4}$ is orthogonal to $\overrightarrow{O9}$ and $\overrightarrow{O10}$, so we must have

$$\overrightarrow{O4} = (\hat{i} + y\hat{j} + xy\hat{k})(1 + y^2 + x^2y^2)^{-1/2}$$
(15.308)

But then, taking the inner product of $\overrightarrow{O1}$ and $\overrightarrow{O4}$, we have at once

$$\cos \theta_{14} = \frac{xy}{\left(\left(1 + x^2 + x^2y^2\right)\left(1 + y^2 + x^2y^2\right)\right)^{1/2}} \\ = \cos\left(\pi/2 - \theta_{12}\right) = \sin \theta_{12}$$
(15.309)

This expression is easily seen to achieve a maximum of 1/3 for $x = y = \pm 1$. So the Kochen-Specker diagram is constructible if

$$0 \le \theta_{12} \le \sin^{-1}\left(\frac{1}{3}\right)$$

Now consider the color map $V: S \to \{red, blue\}$, whose domain is the surface S of the unit sphere, and suppose that V(1) = red and V(2) = blue, then from the Kochen-Specker diagram above, $V(1) = red \to V(7) = V(8) = V(3) = blue$. But V(2) = blue implies that V(4) = red. Hence, V(9) = V(10) = blue. But V(7) = V(9) = blue, which implies that V(5) = red and V(8) = V(10) = blue implies that V(6) = red. But V(5) = V(6) = red is not possible since 5 and 6 are orthogonal directions.

Hence, we conclude there is a minimum angular distance between points of opposite color which is certainly greater than $\sin^{-1}\left(\frac{1}{3}\right)$, otherwise the above contradiction would be derivable.

We now use the lemma to prove the impossibility of the coloring considered in T_3^{real}

Suppose that we take $\theta_{12} = 18^{\circ} < \sin^{-1}(1/3)$, then we know that V(1) = red implies that V(2) = red. But now introduce four additional points, labelled 3,4,5,and 6, lying at 18° intervals along the equator through the points 1 and 2. Then, repeating the above argument

$$V(1) = red \rightarrow V(2) = red \rightarrow V(3) = red \rightarrow V(4) = red \rightarrow V(5) = red \rightarrow V(6) = red$$

But $\theta_{16} = 5 \times 18^\circ = 90^\circ$.

So, if any point on the sphere is colored red, we have demonstrated two orthogonal red points, which contradicts the specification of the coloring.

But, considering any three orthogonal points on the sphere, one of them must be colored red.

Hence, the coloring is not possible, that is, we have demonstrated T_3^{real} .

This argument can be put in the form of a Kochen-Specker diagram with a finite set of vertices which cannot be colored in the specified way.

All we have to do is to choose three arbitrary points p_0, q_0, r_0 and insert the

appropriate fivefold repetition of the Kochen-Specker diagram above, with $\theta_{12} = 18^{\circ}$, between each pair of vertices of the triangle p_0, q_0, r_0 . The resulting beautiful example of an *inconsistent* Kochen-Specker diagram, that is, one which cannot be colored, is shown in Figure 15.14 below.



Figure 15.14: An Inconsistent Kochen-Specker Diagram

Notice that, since a is orthogonal to r_0 and q_0 , as also is p_0 , then we can choose a to coincide with p_0 . Similarly, we can identify b and q_0 and c and r_0 . So the total number of vertices in the diagram is made up of eight vertices in each of the fifteen hexagons with three pairs of vertices identified, leaving $(8 \times 15) - 3 = 117$ distinct vertices.

In other words, what is demonstrated in Figure 15.14 is a collection of 117 points on the unit sphere with the orthogonality relationships indicated, which can be constructed, but which cannot be colored as specified. So we have proved T_3^{real} .

We have shown that if a value function exists for a Hilbert space of a particular dimension N, then it necessarily does so for any space of dimension less than N. Similarly, if a value function exists for a complex Hilbert space, then one exists on any real Hilbert space of the same dimension.

Then, to prove the theorem, it was clear that it suffices to show that no such function can exist in real, 3-dimensional euclidean space.

Reducing the problem in this manner had the advantage that it could be studied in a manifestly geometrical way, in which case it looks like a certain type of map-coloring problem as shown above.

In their original proof, Kochen and Specker found a counter example to the existence of a value function, in the form of a set of 117 vectors in the vector space \Re^3 that could not be consistently assigned the numbers 0 or 1 in the desired way as we have shown above.

This remarkable result shows that a value function $V_{|\psi\rangle}$ cannot exist without violating one of the assumptions implicit in the statement of the theorem. The obvious candidates are:

- 1. The requirement that $V_{|\psi\rangle}(F(A)) = F(V_{|\psi\rangle}(A))$
- 2. The assumption that the quantization map $A \mapsto \hat{A}$ is one-to-one.

The natural situation in which the first requirement might, perhaps, be expected to fail is when we deal with a self-adjoint operator \hat{A} that can be written as functions $\hat{A} = f_1(\hat{A}_1)$ and $\hat{A} = f_2(\hat{A}_2)$ of a pair of self-adjoint operators \hat{A}_1 and \hat{A}_2 with $[\hat{A}_1, \hat{A}_2] \neq 0$.

The value condition implies, in this case, that

$$V_{|\psi\rangle}(F(A)) = f_1(V_{|\psi\rangle}(A_1)) = f_2(V_{|\psi\rangle}(A_2))$$
(15.310)

and, if \hat{A}_1 and \hat{A}_2 do not commute, the wisdom of this assumption could be questioned. For example, if we suppose that the value possessed by a quantity can be found by making an appropriate measurement (which is an assumption, albeit not an unreasonable one), then the last equation implies that measuring \hat{A}_1 and applying f_1 to the result, will yield the same number as measuring \hat{A}_2 and applying f_2 to the result. However, there seems no good reason for supposing this would be so if $[\hat{A}_1, \hat{A}_2] \neq 0$.

On the other hand, dropping the last equation has a very peculiar effect. For example, let \hat{A}_1 and \hat{A}_2 be a pair of non-commuting, self-adjoint operators whose spectral resolutions contain a common projector \hat{P} .

Then \hat{P} can be written as one function of \hat{A}_1 , and as another function of \hat{A}_2 , that is, in general, if a self-adjoint operator \hat{A} has a discrete spectrum with a spectral resolution

$$\hat{A} = \sum_{i=1}^{M} a_i \hat{P}_i \tag{15.311}$$

then the projector \hat{P}_i can be written as a function of \hat{A}

 $\hat{P}_i = \chi_{a_i}(\hat{A}) \tag{15.312}$

where $\chi_r(t) \coloneqq 1$ if t = r and 0 otherwise. Hence, the failure of the value condition P (or equivalently, the truth or falsity of the associated proposition) depends on the *context* in which \hat{P} is taken: if viewed as belonging to the spectral representation of \hat{A}_1 , it will be given one value; if viewed as belonging to that of \hat{A}_2 , it will be given another.

For example, if \hat{P} is thought of as belonging to the spectral representation of \hat{A}_1 , the remaining projectors in the spectral set are a natural choice for commuting partners and, analogously, if \hat{P} is viewed as part of the spectral representation of \hat{A}_2 . More generally, this means that the value of any physical quantity Awhose representing operator \hat{A} has degenerate eigenvalues may depend on the context in which it is considered. In particular, it may depend on the choice of other physical quantities whose associated operators commute with \hat{A} , and which therefore help to label the degeneracy subspaces of \hat{A} .

Yet another way of expressing these ideas is to say that the operator A does not represent a *unique* physical quantity. It has a different meaning depending on what other compatible quantities are considered at the same time. This links up with the second possible way of saving value functions, that is, the idea that the quantization map $A \mapsto \hat{A}$ may be many-to-one.

The Kochen-Specker theorem is not directly relevant to the pragmatic approach to quantum theory in so far as no attempt is made in that approach to think of an individual system as possessing values for its observables. However, if this approach is augmented with the assumptions (1) physical quantities do have values in any individual systems and (2) these values can be revealed by suitable measurements, then the theorem implies that the results obtained will depend on the context in which an observable is studied. In particular, if \hat{A} , \hat{B} and \hat{C} are three operators with

$$[\hat{A}, \hat{B}] = 0 = [\hat{A}, \hat{C}] \quad , \quad [\hat{B}, \hat{C}] \neq 0$$
 (15.313)

then the result of an *individual* measurement of A will depend on whether we choose to measure B or C (or neither) at the same time.

A very important example of this situation arises naturally in the EPR context of a pair of entangled systems that have become spatially separated, and on which measurements are then made in such a way that the measurement events are space-like separated. Remember that two events are space-like separated if no signal can be sent from one to another without exceeding the speed of light and for any such pair of events there is always some inertial frame of reference with respect to which the two events are simultaneous.

If A is associated with the first system and B and C with the second, then we expect to be able to measure A simultaneously with either B or C and hence

$$[\hat{A}, \hat{B}] = 0 = [\hat{A}, \hat{C}]$$
 (15.314)

On the other hand, it is easy to arrange that the operators \hat{B} and \hat{C} associated with the second system are such that $[\hat{B}, \hat{C}] \neq 0$.

Note that the probabilistic predictions of the formalism concerning the results of measuring A do not depend on what else is measured at the same time, that is, the probability of getting result a_m when the state is $|\psi\rangle$ is always just

$$\langle \psi | \hat{P}_m | \psi \rangle \tag{15.315}$$

In addition, statements about the hypothetical values of quantities for individual systems are not amenable to experimental tests. In consequence, the deductions above concerning contextuality will not trouble a pragmatist. Indeed, she may even support them, by citing Bohr's ideas about a property of a quantum system having a meaning only within the context of a specific measurement situation.

However, within a realist interpretation, a contextual assignment of values is in sharp variance with what is normally meant by saying that a property is *possessed*.

In normal discourse, implicit in the statement the quantity A has a value a is an understanding that this is independent of what else might be asserted at the same time. But, according to the Kochen-Specker theorem, in the quantum case we are obliged to talk instead of pairs (A, B) or (A, C) having certain values (a, b) and (a', c) as pairs, and the implication of contextuality is that a may not equal a'.

Note that the analogue of a value-function in a hidden variable theory would involve the assumption that the value of a physical quantity A in a quantum state $|\psi\rangle$ depends on these additional variables. However, this does not change the force of these arguments above.

In particular, it is only in the contextual sense that properties in a hidden variable theory can be said to be *possessed*.

Let make a digression now to consider **quantum logic**.

15.4 The Logic of Quantum Propositions

15.4.1 The Meaning of True

Several times we have mentioned the idea that a projection operator \hat{P} can be regarded as the quantum representative of a proposition \hat{P} , with the eigenvalues 1 and 0 being associated in some way with \hat{P} being true or false respectively. Equivalently, the proposition is represented by the subspace

$$\mathcal{H}_{\hat{P}} \coloneqq \left\{ |\psi\rangle \in \mathcal{H} | \hat{P} | \psi \rangle = |\psi\rangle \right\}$$
(15.316)

of \mathcal{H} . Furthermore, the discussion above showed that, if it existed, a value function $V_{|\psi\rangle}$ satisfying

$$V_{|\psi\rangle}(F(A)) = F(V_{|\psi\rangle}(A))$$
(15.317)

would associate a number 0 or 1 with each projector. The obvious interpretation is that $V_{|\psi\rangle}(P) = 1$ and $V_{|\psi\rangle}(P) = 0$ correspond, respectively, to the proposition being true or false when the quantum state is $|\psi\rangle$.

Binary-valued functions of this type (called *valuations*) play an important role in classical propositional logic, which suggests that it may be profitable to explore quantum theory further from this perspective, particularly the "*logic* of propositions represented by projectors.

A central ingredient will presumably be the fact that each (normalized) state $|\psi\rangle$ gives rise to a probability assignment

$$Prob(P||\psi\rangle) \coloneqq \langle \psi | \hat{P} | \psi \rangle = \langle \psi | \hat{P}^{2} | \psi \rangle$$
$$= (\langle \psi | \hat{P} \rangle (\hat{P} | \psi \rangle) = \| \hat{P} | \psi \rangle \|^{2}$$
(15.318)

which will be interpreted in some way as the probability that the state of affairs represented by \hat{P} is *realized* if the state is $|\psi\rangle$.

Since all propositions in physics can be reduced ultimately to statements about values(possessed, measured or otherwise) of physical quantities, nothing is lost by focussing on this case.

In what follows, we shall only discuss propositions of the type $A \in \Delta$, which asserts that the value of a physical quantity (or easily extended to a finite set of compatible quantities) A lies in some subset $\Delta \subset \mathfrak{R}$ (or will be found to do so if a suitable measurement is made). Assertions of this type refer to the state of affairs at some specific time.

Propositions of the type $A \in \Delta$ are what are normally assumed to be represented by spectral projectors. If the spectrum of \hat{A} is discrete, the operator $\hat{P}_{A\in\Delta}$ is just the sum of the projectors $\hat{P}_{A=a_i}$ where the eigenvalues a_i belong to the subset Δ of real numbers. Of course, a special case is when $\Delta = \{a_j\}$ for some specific eigenvalue a_j , in which case $\hat{P}_{A\in\Delta} = \hat{P}_{A=a_j}$.

The probabilistic predictions of quantum theory are that if the state is $|psi\rangle$, then

$$\operatorname{Prob}\left(A \in \Delta | |\psi\rangle\right) = \left\|\hat{P}_{A \in \Delta} |\psi\rangle\right\|^{2} \tag{15.319}$$

In particular, $Prob(A \in \Delta | |\psi\rangle) = 1$ if and only if $\hat{P}_{A \in \Delta} |\psi\rangle = |\psi\rangle$, that is, $|\psi\rangle$ lies in the eigenspace $\mathcal{H}_{A \in \Delta}(=\mathcal{H}_{\hat{P}_{A \in \Delta}})$ generated by all eigenvectors of \hat{A} whose eigenvalues are in Δ .

Note that a given projection operator may represent more than one proposition of this type. For example, two operators \hat{A} and \hat{B} may share a common spectral projector so that $\hat{P}_{A \in \Delta} = \hat{P}_{B \in \Delta'}$ for some subsets Δ and Δ' of \mathfrak{R} . In this case, we shall say that the propositions $A \in \Delta$ and $B \in \Delta'$ are *physically equivalent*. There are implications for such a definition if $[\hat{A}, \hat{B}] \neq 0$.

Important issues concerning this proposition-projector association include:

- (1) the exact nature of the propositions represented by projection operators
- (2) the way in which the concepts of "*truth* and *falsity* apply to such propositions
- (3) the quantum analogue of the way in which the set of propositions in classical physics acquires the structure of a Boolean algebra from the underlying mathematical representation of states and physical quantities

The nature of the proposition represented by a projection operator depends on the interpretation of quantum theory that is adopted.

A realist might want to say that the projection operator $\hat{P}_{A \in \Delta}$ represents the physical quantity whose value is 1 if the value of A lies in Δ and is 0 otherwise. Hence, in this case, the proposition $A \in \Delta$ is to be read as

The realist version of $A \in \Delta$:

A has a value and this value lies in the subset Δ .

Of course, this leaves open the question of when such an assertion is justified. The situation in classical physics is clear: the proposition is true in a state $s \in S$ if, and only if, $f_A : S \to \Re$ is such that $f_A(s) \in \Delta$. However, as we saw in the Kochen-Specker discussion, any attempt to assign possessed values for all quantities in quantum theory can only be maintained at the expense of considering these properties to be contextual. This means that it is not meaningful to say that any particular proposition is either true or false without specifying what other compatible propositions are to be considered at the same time.

One possibility is to adopt the minimal attitude that a physical quantity A can only be said to have a value a if (1) a is an eigenvalue of \hat{A} and (2) the state $|\psi\rangle$ lies in the associated eigenspace $\mathcal{H}_{A=a}$. One might then argue that, since the first part of the realist version of $A \in \Delta$ is "A has a value.....", the truth of $A \in \Delta$ requires that $|\psi\rangle$ belong to one of the eigenspaces of \hat{A} . Thus, $|\psi\rangle$ must be an eigenvector of \hat{A} . The second part "....... and this value lies in the subset Δ ", then means that the corresponding eigenvalue must belong to the set $\Delta = \{a_1, a_2, \dots, a_d\}$. Note that the first requirement excludes any $|\psi\rangle$ that is the sum of elements in more than one of the eigenspaces $\mathcal{H}_{A=a_1}, \mathcal{H}_{A=a_2}, \dots, \mathcal{H}_{A=a_d}$, even though the formalism gives $Prob(A \in \Delta | |\psi\rangle) = 1$ for all such states. In these circumstances, it is clearly inappropriate to regard the spectral projector $\hat{P}_{A\in\Delta}$ as representing the proposition $A \in \Delta$. Therefore, if one wanted to maintain the proposition-projector link, it would be natural to adopt the weaker condition that $A \in \Delta$ is true in a state $|\psi\rangle$ if $\hat{P}_{A \in \Delta} |\psi\rangle = |\psi\rangle$, that is, if $|\psi\rangle$ is any linear combination of eigenvectors of \hat{A} whose corresponding eigenvalues lie in Δ .

The situation is less ambiguous in the instrumentalist approaches to quantum theory. The projector $\hat{P}_{A \in \Delta}$ now represents a physical observable that is defined operationally by specifying how it is to be measured, that is, measure A, and then, if the result lies in Δ , assign the number 1 to the observable, otherwise assign the number 0. The proposition $A \in \Delta$ should now be read as asserting that a *measurement* of A will yield a result that lies in the subset Δ .

On the face to it, the statement "if a measurement of A is made, then the result will lie in Δ " is applicable to a single system, as is the realist claim that "Ahas a value that lies in Δ ". However, the instrumentalist form of the proposition is not a statement about how things are, but rather a claim about what would happen *if* a certain operation was performed. This seems to cry out for a positivist-type verification, that is, make the measurement and see what happens - if the result does not lie in Δ , then the proposition is certainly false.

But what if the result *does* lie in Δ ? Does this mean this proposition is true? Certainly not if, as is arguably the case, a more precise rendering of the proposition is:

The modal version of $A \in \Delta$:

if a measurement of A is made, then, necessarily, the result will lie in the subset Δ .

Put in the modal form, the proposition is manifestly counterfactual and cannot be verified by any single, or finite set, of measurements. Indeed, it could be argued that, in this form, the proposition does not apply at all to an individual system but only to a collection of such on which repeated measurements are to be made. Thus, in this reading, it is consistent to say that states and propositions apply only to such collections.

The discussion above shows why, in the relative-frequency, anti-realist interpretations of quantum theory, we are lead naturally to read the proposition $A \in \Delta$ as:

The probability-one version of $A \in \Delta$:

if a measurement of A is made, then, with, probability one, the result will lie in the subset Δ . in which case it is clear when it would be asserted as true, namely,

if the quantum state is $|\psi\rangle$, a proposition T represented by a projection operator \hat{P}_T is true if $Prob(T||\psi\rangle) = 1$

Some Comments on these Ideas

1. Since

$$Prob(T||\psi\rangle) = \|\hat{P}_T|\psi\rangle\|^2$$

the condition $Prob(T||\psi\rangle) = 1$ implies that $\hat{P}_T |\psi\rangle = |\psi\rangle$, that is, $|\psi\rangle$ is, in fact, an eigenvector of \hat{P}_T with eigenvalue 1.

- 2. This result implies that the proposition $A \in \Delta$ is true in any state $|\psi\rangle$ that can be written as a linear superposition of the eigenvectors associated with the eigenvalues in Δ . Of course, this does *not* mean that the probability of getting any *specific* eigenvalue is equal to 1. Indeed, this number will be strictly less than 1 if $|\psi\rangle$ has non-zero expansion coefficients for more than one of the eigenspaces. Note that, unlike in the realist case, this causes no problems, since the modal form of $A \in \Delta$ does not say that a measurement of A necessarily gives any one particular element of Δ .
- 3. Care must be taken when handling propositions in this modal form. For example, if the proposition $A = a_m$ is interpreted as "if A is measured, then the result will necessarily be a_m ", then the value of $Prob(A = a_m ||\psi\rangle)$ cannot be read as the probability that the proposition is true when the state is $|\psi\rangle$. Rather, $Prob(A = a_m ||\psi\rangle)$ refers to the relative frequency with which result a_m will be found on a given collection of systems.

For example, the statement "there is a 70% chance that the proposition "if A is measured, then the result will necessarily be a_m is true", is quite different from "if A is measured, then there is a 70% chance that the result will be a_m ". It is the latter that is intended in the quantum formalism by the statement $Prob(A = a_m ||\psi\rangle) = 0.7$. Note that, if desired, one might introduce an extended class of modal propositions of the form

if a measurement of A is made, then the probability that the result will lie in Δ IS r.

where the real number r satisfies $0 \le r \le 1$. The special value r = 1 then corresponds to the probability-one proposition above.

15.4.2 Is "False" the Same as "Not True"?

The next issue to consider is what it means to say that a proposition is *false* and under what circumstances in quantum theory such an assertion would be justified.

In *classical physics or logic*, this causes no difficulties:

a proposition is false if and only if it is not true

If we adopt this idea in quantum theory then, in the relative-frequency interpretations, " $A \in \Delta$ is false" means that, in a long series of repeated measurements of A, one or more numbers not lying in Δ will occur with a non-zero relative frequency. In general, this suggests the definition that a proposition T is "false" in a state $|\psi\rangle$ if $Prob(T||\psi\rangle) < 1$.

On the other hand, a realist may balk at the idea that the proposition $A \in \Delta$ could be said to be false if there is still a non-zero probability of *finding* values in Δ . When confronted with the existing formalism of quantum theory - in particular the idea that propositions are to be associated with projection operators - a realist may feel that the most natural assignment of truth and falsity in a state $|\psi\rangle$ is that a proposition $A \in \Delta$ is (1) true in state $|\psi\rangle$ if $Prob(A \in \Delta ||\psi\rangle) = 1$ (that is, $|\psi\rangle \in \mathcal{H}_{A \in \Delta}$) and (2) false if $Prob(A \in \Delta ||\psi\rangle) = 0$ (that is, $|\psi\rangle \in \mathcal{H}^{\perp}_{A \in \Delta}$).

However, any vector $|\psi\rangle \in \mathcal{H}$ can be written as a sum of components in $\mathcal{H}_{A\in\Delta}$ and $\mathcal{H}_{A\in\Delta}^{\perp}$, and, according to these assignments, the proposition $A \in \Delta$ cannot be said to be either true *or* false if both components are non-zero. This suggests that some sort of multi-valued logic should be used. The simplest such attempt, due to Reichenbach is to use a three-valued logic in which a proposition can be either true, false, or indeterminate. The typical quantum mechanical situation in which a non-trivial superposition of eigenvectors leads to a proposition being neither true nor false would then be assigned to the indeterminate category.

A more complex possibility is to use a continuous spectrum of truth values lying between 0 and 1, with the truth value of the proposition T in a state $|\psi\rangle$ being set equal to $Prob(T||\psi\rangle)$. This is the idea that lies behind the concept of fuzzy logic.

But, in either case, it is not really clear what the meaning is of a proposition that is deemed to apply to a single system but which is then said to be neither true nor false. Philosophers have debated this for some time without reaching any definite conclusions.

In addition, serious worries have been expressed about using the idea of using a multi-valued logic within a mathematical framework that is, itself, based firmly on classical two-valued logic.

Another major problem with multi-valued logics is to decide on the appropriate analogues of the usual logical connectives *and*, *or*, *negation*, and *logical implication* that are usually introduced in the context of classical physics. Many mathematical attempts have been tried, but no clear consensus has emerged. The difficulties with logical connectives can be alleviated by adopting the strategy in which a proposition $A \in \Delta$ is understood to be false in state $|\psi\rangle$ if it is not true, that is, if $Prob(A \in \Delta | |\psi\rangle) < 1$. This approach is quite natural in instrumentalist interpretations of quantum theory, and results in a two-valued propositional structure, albeit at the expense of introducing a certain asymmetry between the concepts of "true" and "false". It is still necessary to define the logical connectives, however.

The Logical Connectives

The construction of a quantum logic on the set of two-valued (true/false) propositions originally started by Birkhoff and von Neumann. They started with the set $\wp(\mathcal{H})$ of all closed subspaces of a Hilbert space \mathcal{H} (or, equivalently, with the set of all projection operators) and suggested certain analogues of the classical logical operations. The basic definitions are as follows.

1. A proposition T implies another U, written $T \leq U$, if for all states $|\psi\rangle$ such that $Prob(T||\psi\rangle) = 1$, we have $Prob(U||\psi\rangle) = 1$, that is, U is true in all states in which T is true. This is equivalent to \mathcal{H}_T being a closed subspace of \mathcal{H}_U .

The analogous classical relation is $S_T \subset S_U$.

If \hat{P}_T and \hat{P}_U are the associated projection operators, the relation $T \leq U$, is equivalent to

$$\hat{P}_T \hat{P}_U = \hat{P}_U \hat{P}_T = \hat{P}_T \tag{15.320}$$

Note that if T implies U and U implies T, it is natural to say that the propositions T and U are equivalent. Indeed, The former means $\hat{P}_T \hat{P}_U = \hat{P}_T$ and $\hat{P}_T \hat{P}_U = \hat{P}_U$, that is, $\hat{P}_T = \hat{P}_U$, which is the definition of physical equivalence suggested earlier. As is the case in classical physics, the appropriate objects to study are the equivalence classes of propositions which, in the quantum case, are the projection operators. This means that it is more appropriate to view the logical operations as defined on projection operators (or, equivalently, topologically closed subspaces), than on propositions, per se.

2. The operator that corresponds to the *identically false* proposition is the null operator $\hat{\varphi}$ that maps every vector in \mathcal{H} to the null vector, and the operator that is the identically true proposition is the unit or identity operator \hat{I} . Thus, for any projection operator \hat{P} , we have $\hat{\varphi} \leq \hat{P} \leq \hat{I}$.

In classical physics, the analogue of these two propositions are the empty set \emptyset and the whole space S respectively, and for all subsets S_T of S we have $\emptyset \subset S_T \subset S$.

3. If T is a proposition, the proposition $\neg T$ (not T) is defined by requiring that, for all states $|\psi\rangle$, $Prob(\neg T||\psi\rangle) = 1$ if, and only if, $Prob(T||\psi\rangle) = 0$.

This is equivalent to the relation $\mathcal{H}_{\neg T} = (\mathcal{H}_T)^{\perp}$. This relation determines a unique projection operator $\hat{P}_{\neg T}$ that represents $\neg T$:

$$\hat{P}_{\neg T} = \hat{I} - \hat{P}_T$$
 (15.321)

which actually implies the (superficially stronger) relation between the probabilities of T and $\neg T$

$$Prob(T||\psi\rangle) + Prob(\neg T||\psi\rangle) = 1$$
(15.322)

The classical analogue is $S_{\neg T} = S - S_T$.

Unlike the classical case, the quantum definition has the peculiar property that T can be *false* in a state $|\psi\rangle$ (that is, T is not true, so that $Prob(T||\psi\rangle) < 1$) without implying that $\neg T$ is *true* (which requires that $Prob(T||\psi\rangle) = 0$). But, as expected, $\neg T$ true *does* imply that T is false! This curious asymmetry stems directly from (1) the existence of linear superpositions of eigenstates of the operator \hat{P}_T and (2) our desire to have a binary-valued, rather than trinary-valued, logic.

4. Let T and U be a pair of propositions with associated closed subspaces \mathcal{H}_T and \mathcal{H}_U , and projection operators \hat{P}_T and \hat{P}_U , respectively. Then the proposition $T \wedge U$ (to be interpreted as some type of conjunction, T AND U) is defined by requiring that $Prob(T \wedge U | |\psi\rangle) = 1$ in a state $|\psi\rangle$ if and only if $Prob(T | |\psi\rangle) = 1$ and $Prob(U | |\psi\rangle) = 1$, that is, $T \wedge U$ is true in the state $|\psi\rangle$ if and only if both T AND U are true. This means

$$\mathcal{H}_{T \wedge U} = \mathcal{H}_T \cap \mathcal{H}_U \tag{15.323}$$

which is reminiscent of the classical result $S_{T \wedge U} = S_T \cap S_U$.

Expressed in terms of subspaces, the quantum definition seems rather natural. However, there is no simple way of translating it into the language of projection operators since the operator $\hat{P}_T \wedge \hat{P}_U := \hat{P}_{T \wedge U}$ that projects onto $\mathcal{H}_T \cap \mathcal{H}_U$ is not a simple function of the projection operators \hat{P}_T and \hat{P}_U . If $[\hat{P}_T, \hat{P}_U] = 0$ it can be shown that the projection operator $\hat{P}_T \wedge \hat{P}_U$ that represents the proposition $T \wedge U$ is

$$\hat{P}_T \wedge \hat{P}_U = \hat{P}_T \hat{P}_U \tag{15.324}$$

5. In classical physics, the set that represents the disjunction $T \vee U$ ($T \ OR \ U$) of a pair of propositions T and U, is the union $S_T \cup S_U$ of the sets S_T and S_U that represent them, that is, it is the smallest subset of the state space S that contains both S_T and S_U .

The obvious analogue in quantum theory is the set $\mathcal{H}_{T \vee U}$ equal to the union of \mathcal{H}_T and \mathcal{H}_U . But this cannot be correct since $\mathcal{H}_T \cup \mathcal{H}_U$ is not a *linear* subspace of \mathcal{H} , that is, it is not closed under the operation of taking

sums of vectors. This suggests that the more appropriate definition would be $\mathcal{H}_{T \vee U} = \mathcal{H}_T + \mathcal{H}_U$, which is defined to be the linear sum of all vectors in \mathcal{H}_T and \mathcal{H}_U . However, even this is not correct if \mathcal{H} has an infinite dimension since then $\mathcal{H}_T + \mathcal{H}_U$ may not be topologically closed. This defect is remedied by the final definition

$$\mathcal{H}_{T \vee U} = \overline{\mathcal{H}_T + \mathcal{H}_U} \tag{15.325}$$

which is the smallest, topologically closed linear subspace of that contains both \mathcal{H}_T and \mathcal{H}_U .

As in the case of the conjunction, there is no easy way to write this last relation in terms of the associated projection operators. However, if $[\hat{P}_T, \hat{P}_U] = 0$, then the projection operator $\hat{P}_T \vee \hat{P}_U \coloneqq \hat{P}_{T \vee U}$ that represents the proposition $T \vee U$ is

$$\hat{P}_T \vee \hat{P}_U = \hat{P}_T + \hat{P}_U - \hat{P}_T \hat{P}_U \tag{15.326}$$

In particular, if $\hat{P}_T \hat{P}_U = 0$ then $\hat{P}_T \vee \hat{P}_U = \hat{P}_T + \hat{P}_U$ (this is the classical result).

Some Comments

1. The closed subspaces \mathcal{H}_T and \mathcal{H}_U of \mathcal{H} satisfy the equation

$$\overline{\mathcal{H}_T + \mathcal{H}_U} = (\mathcal{H}_T^{\perp} \cap \mathcal{H}_U^{\perp})^{\perp} \tag{15.327}$$

This is the analogue of the DeMorgan rule of classical set theory

$$S_T \cup S_U = S - ((S - S_T) \cap (S - S_U))$$
(15.328)

which corresponds to the logical identity $T \lor U = \neg(\neg T \land \neg U)$.

This fact provides further justification for the consistency of the above assignments of logical connectives.

2. Care must be taken in interpreting the assignment of logical connectives. This is particularly true of the idea of " $T \wedge U$ ". One may interpret \wedge as "and" in the normal sense only if the two operators commute since, as mentioned earlier, only then is it unequivocally meaningful to assert that states of the system exist in which both properties are possessed at the same time. In the non-commuting case, the best that can be said (instead of

$$\hat{P}_T \wedge \hat{P}_U = \hat{P}_T \hat{P}_U \tag{15.329}$$

is that

$$\hat{P}_T \wedge \hat{P}_U = \lim_{k \to \infty} \left(\hat{P}_T \hat{P}_U \right)^k \tag{15.330}$$

which is sometimes read as saying that $T \wedge U$ refers to the results of an infinite sequence of measurements of T and U.

3. The fact that most pairs of operators do *not* commute is reflected in the crucial property of the set of quantum propositions that the algebraic structure associated with the definitions of \wedge and \vee fails to be distributive.

This can be seen easily with the aid of a simple example. Let $\mathcal{H}_{|\psi_1\rangle}$ and $\mathcal{H}_{|\psi_2\rangle}$ be one-dimensional subspaces of a two-dimensional Hilbert space \mathcal{H} , spanned by (that is, all complex multiples of) the linearly-independent vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ respectively, and let $|\phi\rangle$ be any non-trivial linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$. Then we have

$$\mathcal{H}_{|\phi\rangle} \cap \left(\mathcal{H}_{|\psi_1\rangle} + \mathcal{H}_{|\psi_2\rangle}\right) = \mathcal{H}_{|\phi\rangle} \cap \mathcal{H} = \mathcal{H}_{|\phi\rangle} \tag{15.331}$$

but if we use the standard distributive property we have

$$\mathcal{H}_{|\phi\rangle} \cap \left(\mathcal{H}_{|\psi_1\rangle} + \mathcal{H}_{|\psi_2\rangle}\right) = \mathcal{H}_{|\phi\rangle} \cap \mathcal{H}_{|\psi_1\rangle} + \mathcal{H}_{|\phi\rangle} \cap \mathcal{H}_{|\psi_2\rangle} = \mathcal{H}_{\varnothing} + \mathcal{H}_{\varnothing} = \mathcal{H}_{\varnothing} \quad (15.332)$$

We thus have the contradiction $\mathcal{H}_{|\phi\rangle} = \mathcal{H}_{\varnothing}$. This result contrasts sharply with the distributive property of classical propositions, which is direct consequence of the Boolean nature of the algebra if intersections and unions of subsets of a classical state space.

Most of the strange, non-classical features of quantum theory can be traced back to this non-distributive property of the logical structure of quantum propositions.

It is useful to think about Gleason's theorem in light of these discussions.

Gleason's Theorem

The probability rules for density matrices imply that for any proposition P, with associated projector $\hat{P} \in \wp(\mathcal{H})$, the probability associated with P in the state $\hat{\rho}$ is

$$Prob(P|\rho) = Tr\left(\hat{\rho}\hat{P}\right) \tag{15.333}$$

An interesting and important question arises at this point. Are there any other ways of assigning probabilities to the elements of $\wp(\mathcal{H})$, or, is the standard quantum formalism unique? More precisely, can we find a new probabilistic theory by starting with some Hilbert space \mathcal{H} , with its non-distributive algebra $\wp(\mathcal{H})$ of subspaces/projection operators, and then construct a probability map $Prob : \wp(\mathcal{H}) \to \Re$ that is *not* of the type given above? In particular, what is the space of states in such a theory?

To tackle this question we must first decide what requirements should be satisfied by a *probability map* $Prob : \wp(\mathcal{H}) \to \mathfrak{R}$. The analogous question in classical statistical physics is answered by defining a general *probability measure* to be a
real-valued function μ of subsets of S that satisfies the three conditions

$$\label{eq:prod} \begin{array}{l} 0 \leq \mu(W) \leq 1 \mbox{ for all such subsets } W\\ \mu(\varnothing) = 0 \quad , \quad \mu(S) = 1\\ \mu(W_1 \cup W_2 \cup \ldots) = \mu(W_1) + \mu(W_2) + \ldots .. \end{array}$$

In the quantum case, one obvious condition is $0 \leq Prob(P) \leq 1$ for all propositions $P \in \wp(\mathcal{H})$. Two other, essentially trivial, requirements are $Prob(\emptyset) = 0$ and Prob(I) = 1, where \emptyset and I correspond respectively to the propositions that are identically false and true.

They key question is what should be required of the probabilities $Prob(T \wedge U)$ and $Prob(T \vee U)$ for a pair of propositions T and U.

It is helpful to start by considering the analogous question in classical physics, where propositions correspond to subspaces of the state space S. In this case, bearing in mind that $S_{T \wedge U} = S_T \cap S_U$ and $S_{T \vee U} = S_T \cup S_U$, it is easy to see with the aid of a Venn diagram that one required condition is

$$Prob(T \lor U) = Prob(T) + Prob(U) \tag{15.334}$$

which, if $\{P_1, P_2, ..., P_M\}$ is any finite set of propositions that are pairwise exclusive, generalizes at once to

$$Prob(P_1 \lor P_2 \lor \dots \lor \lor P_M) = \sum_{i=1}^M Prob(P_i)$$
(15.335)

An important technical requirement in classical probability theory is *countable* additivity, that is, this relation should continue to hold in the limit $M \to \infty$.

The quantum analogue of two mutually-exclusive propositions is a pair of projection operators \hat{P}_T , \hat{P}_U that are orthogonal, that is, $\hat{P}_T\hat{P}_U = 0 = \hat{P}_U\hat{P}_T$. In this case, problems of incompatibility do not apply, and it is natural to suppose that the last relation passes across in the form

$$\hat{P}_1 \vee \hat{P}_2 \vee \dots \vee \hat{P}_M = \sum_{i=1}^M \hat{P}_i$$
 (15.336)

for any collection of pairwise orthogonal projection operators.

Thus, a minimal set of requirements on any quantum probability function $Prob: \wp(H) \to \Re$ is

$$0 \le Prob(\hat{P}) \le 1 \text{ for all } \hat{P} \in \wp(\mathcal{H})$$
$$Prob(\hat{0}) = 0 \quad , \quad Prob(\hat{I}) = 1$$
$$Prob\left(\sum_{i=1}^{\infty} \hat{P}_i\right) = \sum_{i=1}^{\infty} Prob(\hat{P}_i)$$

for any finite or countably infinite set $\{P_1, P_2, ...\}$ of projection operators that are pairwise mutually orthogonal.

Typically, such sets arise as the spectral projectors of a self-adjoint operator.

One way of satisfying these relations is to define

$$Prob(\hat{P}) = Tr(\hat{\rho}\hat{P}) \tag{15.337}$$

where $\hat{\rho}$ is any density operator.

12pt] A remarkable theorem due to Gleason shows that, provided that $dim(\mathcal{H}) > 2$, the converse is true - the only way of satisfying

$$0 \le Prob(\hat{P}) \le 1 \text{ for all } \hat{P} \in \wp(\mathcal{H})$$
$$Prob(\hat{0}) = 0 \quad , \quad Prob(\hat{I}) = 1$$
$$Prob\left(\sum_{i=1}^{\infty} \hat{P}_i\right) = \sum_{i=1}^{\infty} Prob(\hat{P}_i)$$

is with the aid of a density operator and the relation

$$Prob(\hat{P}) = Tr(\hat{\rho}\hat{P}) \tag{15.338}$$

Gleason's theorem places strong constraints on any attempts to modify the standard quantum formalism as, for example, might be desired in the construction of hidden variable theories. It also gives a rather deep reason why density operators play such an important role in quantum theory.

15.5 Quantum Mechanical Picture of the World

Let us look at Kochen-Speker and Gleason in another way to help our understanding. Quantum mechanics provides us with the most detailed picture of the natural world. The mention of quantum mechanics conjures up ideas of uncertainty, indeterminacy, and probability. This section aims to explain these ideas which based on the knowledge we have gained in this text.

If you look at most papers on this subject it seems that only the experts can know the details, because only they have the knowledge of the esoteric mathematics required. Hopefully we can simplify the arguments using only elementary mathematics(especially geometric arguments) in this presentation.

We first build a mathematical model of the subatomic world based on the properties revealed by the Stern-Gerlach experiment. We then analyze the model and prove a theorem whose physical implications are immediately obvious. One must follow the reasoning carefully and analyze the figures to understand the proof of the theorem. We will find that the subatomic world cannot be completely determined and that its properties cannot be definite before an experiment reveals these properties to us.

15.5.1 The Model

To understand atoms or subatomic particles, the tools of classical physics, as we have seen, are not sufficient. We need new kinds of concepts and laws, which are contained in quantum mechanics. Because matter and radiation consists of subatomic particles, the macroscopic world must be ultimately explained according to quantum principles.

As we saw earlier, one of the first surprising results on the behavior of small particles was observed by Stern and Gerlach in 1922. In that experiment, a beam of silver atoms was sent through a magnet as shown in Fig. 15.15 below.



Figure 15.15: Stern-Gerlach Setup

According to classical mechanics, the silver atoms should be deflected by a certain angle. There should be a large range of scattering angles and, therefore, a band of impacts on a screen placed behind the magnet. Surprisingly, only two narrow strips were observed, one above the initial direction and one below. The fact that only two strips were obtained was totally unexpected in the context of classical physics; the only explanation of this fact was that a property of the silver atoms-called intrinsic angular momentum or spin-could take on only two possible values, $\pm \hbar/2$. More precisely, the projection of the spin along the direction of the magnetic field can have only two values in this case.

It was subsequently discovered that for atoms other than silver, the beam split into three, four, or more branches, depending on the kind of atom. If the beam of particles splits into two branches, we say the particle has spin 1/2; if it splits into three, we say the particle has spin 1; if it splits into four, we say the particle has spin 3/2, and so forth.

The discovery of angular momentum quantization was a key moment in the creation of quantum mechanics. We are interested only in a particular aspect of the Stern-Gerlach experiment. In fact, we will not even talk directly about the angular momentum, although it will constantly enhance the argument. Let us consider spin 1 particles. If we shoot a beam of those particles at a Stern-Gerlach device positioned according to Fig. 15.16 (oriented in the z-direction represented by the unit vector \hat{z}), some of the particles will deflect up (in state $|1_z\rangle = |\uparrow_z\rangle$), some of them down(in state $|-1_z\rangle = |\downarrow_z\rangle$), and a third group will not deflect up or down(in state $|0_z\rangle = |\rightarrow_z\rangle$).



Figure 15.16: Stern-Gerlach oriented in z-direction

If the magnet is turned to face in any other direction, say the -x-direction represented by the unit vector \hat{x} , as in Fig. 15.17 below



Figure 15.17: Stern-Gerlach oriented in -x-direction

the result will be the same: a beam goes to the right, another one goes to the left, and a third beam is not deflected. The corresponding states are $|1_x\rangle = |\uparrow_x\rangle$, $|-1_x\rangle = |\downarrow_x\rangle$, and $|0_x\rangle = |\rightarrow_x\rangle$ as before.

From this experiment, we come to the important conclusion that the state of a system is characterized by a state vector that is labeled by a number or an arrow representing a direction in space. This type of characterization, as we have seen, turns out to be a basic principle of quantum mechanics.

We can use a Stern-Gerlach device to answer the following question: Is the system in the $|0_x\rangle = |\rightarrow_x\rangle$ state? The answer will be yes for the beam that does not deflect when the magnetic field points in the *x*-direction. The beams that are deflected will give us negative answer to this question. This kind of question, which is answered with only two alternatives: yes or no, 1 or 0, is called a *projector*. Thus, the question, *Is the system in the* $|0_x\rangle = |\rightarrow_x\rangle$ state? is called the \leftarrow_x or 0_x projector (or projection operator) and is represented by the operator symbol P_{\leftarrow_x} or P_{0_x} . In the same way, we can apply a 0_y projector P_{0_y} which corresponds to the question, *Is the system in the* $|0_y\rangle = |\rightarrow_y\rangle$ state? In general, we can define the projector P_{0_n} corresponding to an arbitrary direction represented by the unit vector \hat{n} .

But quantum mechanics, as we have seen, is very peculiar. Suppose that we apply the projector P_{0_x} with an affirmative response, so that we are sure that the system (the atom) is in the $|0_x\rangle$ state. If we now introduce a second Stern-Gerlach magnet, pointing in any other direction \hat{n} , then the projector P_{0_n} will be answered sometimes affirmatively and sometimes negatively. To be precise, the probability of obtaining yes is equal to the square of the projection (probability amplitude) of \hat{n} on \hat{x} , i.e., $\hat{n} \cdot \hat{x}$ as shown in Fig. 15.18 below.

This, as we know, is the same as the square of the scalar product (probability amplitude) of the states representing the atom in each case, i.e., $\langle 0_n | 0_x \rangle$, which is just the Born Rule. If the direction \hat{n} is orthogonal to \hat{x} , then the projection is zero. Therefore, the probability that the system is in the $|0_n\rangle$ is zero. In this



Figure 15.18: Projection = Probability Amplitude

case, the answer to the question P_n will be no if P_x had been affirmative.

Gleason, in his remarkable theorem published in 1957 (A. Gleason, "Measures on the closed subspaces of a Hilbert space," J. Math. Mech. 6(6), 885-893 (1957)), proved that a probability measure μ defined over a spherical surface [or a linear space of dimension 3 if for any vector a' and any number λ , $\mu(a) = \mu(\lambda a)$ (a and λa are the same physical state)] has to be of the form: $prob(P_{\theta} = 1|P_z = 1) = \cos^2 \theta$. (Note: $P_{\theta} = 1$ is a convenient way of saying that P_{θ} takes on the value 1. Other authors write $v(P_{\theta=1} \text{ instead})$. Gleason showed the equivalent result for any dimension of Hilbert space.

Questions referring to perpendicular directions are mutually exclusive: if one of them is affirmative, the other will be negative. Because these questions or projectors do not interfere with each other, we say that they are compatible, in the sense that they can be measured together. (If the directions are not perpendicular, they can interfere: we can obtain two affirmative results). Mathematically this looks like:

$$|0_x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\-1 \end{pmatrix} \quad |0_y\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\1 \end{pmatrix} \quad |0_z\rangle = \begin{pmatrix} 0\\1\\0 \end{pmatrix}$$

Thus,

$$\langle 0_x | 0_y \rangle = \langle 0_x | 0_z \rangle = \langle 0_y | 0_z \rangle = 0$$

In three-dimensional space, there are at most three compatible projectors. For example, the projectors, P_{0_x} , P_{0_y} , and P_{0_z} are compatible, because they do not interfere with each other and can be implemented at the same time, meaning that the response will be yes for one of the three and no for the other two. If the system is in the $|0_x\rangle$ state, for instance, it cannot be in the $|0_y\rangle$ state or the $|0_z\rangle$ state.

In general, a set of three directions that are mutually perpendicular will be

called an orthogonal triple. In an orthogonal triple, one of the projectors will yield yes (1) and the other two will yield no (0). The maximum number of compatible projectors is three because we are considering a spin-1 particle. The spin of other kinds of particles as well as other quantum observable quantities will require a different number of dimensions. But the important point is that any quantum observable quantity can be split into projectors so that our analysis can be extended to every quantum observable quantity.

15.5.2 The Question

With these ideas in mind, we turn our attention to the central idea of this section: What picture of the world does quantum mechanics provide? We know quantum mechanics is a probabilistic theory. In each experiment we have a certain probability of obtaining one result or another. But when we throw a die, we also obtain a result with a certain probability. Is it the same kind of randomness? Do the probabilities have the same nature in both cases?

When we throw the die, we could in principle know what number we would see if we knew the precise value of the force applied to the die. But there are so many elements we do not control that we accept the result as a random event, even though in theory, we could predict the result if we analyzed the details of the enormous variety of variables that are relevant. We use probabilities because analyzing all those details would be too laborious. It is a question of practical difficulty; not just of principle.

What would happen in a quantum experiment? Would there be any way of determining the result of an experiment through a complete understanding of the variables? We know that when we repeat a quantum experiment we can obtain different results, even with the same initial conditions. That does not happen in the case of the die: if the forces were the same, the result would be the same as well. In a quantum experiment we may need to have more profound knowledge. Moreover, it is possible that today's technology is insufficient to discover the subtle variables that cause the same experiment to produce different results. Is it not plausible to think that there should be something within the system that explains why we obtain one result and not another? Einstein, among others, thought this way. For him, quantum mechanics-despite its achievements-seemed to be an incomplete theory because it could not predict with certainty the result of an experiment. Even though our insufficient knowledge prevents us from identifying it, could each object have a hidden variable that could explain its apparently random behavior in a particular experiment? Or do we have to admit that quantum uncertainty is more radical? Is matter really intrinsically random so that there is no possibility, even in principle, of predicting the result of an experiment?

An alternative lies between these two pictures of the world. If the hidden variables explaining the apparently random results exist, we would have a totally deterministic world. It is a world where there is a cause for everything that happens. In such a world of hidden variables, the properties of a subatomic particle, or any other quantum system, would be clearly defined. If we return to the set of projectors we have constructed, then each projector would have a plain answer: yes (1) or no (0). As we have said the projectors take on only two values, 0 or 1, with a certain probability. When we say that the projectors are defined, we mean that they take on the value 1 (or 0) with probability 1. Therefore the expectation value of any projector in that case is $\langle P_{theta} \rangle = prob(P_{\theta} = 1) = 0$ or 1. In brief definite values' means $\langle P_{theta} \rangle = 0$ or 1. If there were a definite world out there, we could ascribe the values 0 or 1 to all the projectors, with the condition that if three projectors are mutually orthogonal, only one of them will be ascribed the value 1. Note that the assumption $\langle P_{theta} \rangle = 0$ or 1 is by itself contradictory to quantum mechanics because in the latter $prob(P_{\theta} = 1 | P_z = 1) = \cos^2 \theta$. We do not have to wait for the conclusion of the theorem. It is a matter of principle: a theory with definite values clashes with quantum mechanics. So for that matter we do not need the KSB theorem. The merit of the theorem is to show that any theory with definite values and satisfying $prob(\sum P_i) = \sum prob(P_i)$ (P_i mutually orthogonal) is contradictory by itself.

But this proposition is a mathematical one and can be analyzed as such. Thus, mathematics will tell us which is the correct picture of the world. (This power of mathematics is possible only because we have previously constructed the projectors, a mathematical structure, superimposed on the physical world).

In 1932 the problem of hidden variables was discussed by Von Neumann. He presented it like this: Suppose that the correct picture of the world is the first one; that is, let us suppose that apparently identical states have a hidden variable that makes them different. Then we could select a set of systems that were exactly in the same pure state, that is, with the same value for the hidden variable. In this case, our set would be a true dispersionless state (dispersion is the deviation from the mean). On the contrary, if there were no hidden variables, then apparently identical systems (systems that are in the same state) would have slight differences which would correspond to their different behavior in the experiments; thus, they do show dispersion. Von Neumann proved that there are no dispersionless states; therefore there cannot be hidden variables. But his demonstration was not conclusive. The matter was not resolved until 1966-1967.

It was Bell, who used a result obtained previously by Gleason and Kochen and Specker, who proved that there cannot be pure dispersionless states, that is, it is impossible to ascribe values 0, 1 to the projectors consistently. We present here a simplified version, proposed by Gill and Keanes (and based on the work of Piron).

As we have said, the question is whether it is possible to maintain a world picture in which the quantum observable quantities, the properties of subatomic particles, exist before we measure or look at them (looking at things is a way of measuring them). In that world we could assign values to every projector.

Because the projectors point in any direction of space, we can talk about projectors or directions alike. Besides, let us remember that, if we consider a sphere of unit radius, each direction has one corresponding point on it: the one where that direction goes through the sphere. Thus we can equally well speak of projectors, directions, or points on a sphere. Consequently, the existence of an outside world, determinate and deterministic, would mean that we can ascribe values 0 or 1 to all the points on a sphere. But remember that we have a restriction: in each orthogonal triple, we ascribe the value 1 to only one point and the 0 to the other two.

To see whether it is possible to assign values 0 or 1 to all the points on a spherical surface with that restriction, we need a geometrical lemma.

15.5.3 The Geometrical Lemma

Let us now look at the orthogonal triple A, A_E, A_P as shown in Fig.15.19 below.



Figure 15.19: Orthogonal Triple

We have rotated the equatorial plane so that the great circle has A as its most northerly point, and crosses the equator at the point A_E . Call A_P the point of the northern hemisphere orthogonal to that great circle. Of these three points, one must have the value 1; the other two, 0.

Proposition - If the value of A_P , a direction perpendicular to a great circle, is 1, then all the directions in the great circle have to take on the value 0.

To see that this statement is true, it is sufficient to note that any direction B in the great circle can make up an orthogonal triple with A_P and another direction B' in the circle, perpendicular to B as shown in Fig.15.20 below.

Because an orthogonal triple can have only one 1, B and B^\prime must take on the value 0.



Figure 15.20: If value of A_P is 1, B and B' take on the value 0

We next prove a lemma which will be fundamental to our argument.

Proposition - Starting from one point A of the northern hemisphere, we can reach any more southerly point than A by a finite sequence of great circle descents.

The great circle descent from a point A is the great circle which has A as its most northerly point. (From now on, the great circle descent from A will be called the great circle from A). Beginning at any point A (not at the north pole or on the equator), we can descend along the great circle from A to another point B; then we can descend along the great circle from B to another point C; we can once more descend along the great circle from C; and so forth. The lemma states that we can go along great circle descents from one point to another further south. That means that we can travel from Madrid to Manila going along a sequence of great circle descents.

The proof of this lemma is straightforward if we project the points of the northern hemisphere from the center of the sphere onto the plane tangent to the sphere at the north pole. In Fig.15.21 below we see that the projection of a parallel is a circumference (parallels are lines of constant latitude). We also see that a great circle descent projects onto a straight line, the tangent to the circumference projected by the parallel that contains the summit of the great circle. Besides, the meridians give rise to straight lines passing through the north pole.

These considerations imply that the great circle descent from S projects onto a straight line, tangent to the circumference at the point s of the tangent plane and perpendicular at that point to the line projected by the meridian. To prove the lemma, we begin with the simplest case: How can we go along great circle descents from the point S to the point T, both on the same meridian (see Fig.15.22 below)?



Figure 15.21: Parallel and great circle that are tangent at S project from sphere center onto tangent plane at North Pole, giving rise, respectively, to a circumference and a straight line tangent to it at point s. Point C of great circle from S projects onto point c of straight line. Meridian through S gives rise to straight line PS, perpendicular to straight line sc.



Figure 15.22: S and T are on the same meridian

First, let us project the points S and T onto the plane tangent to the sphere at the north pole (see Fig.15.23 below)

We will obtain the points s and t. We also project the great circle from $S(D_S)$ and obtain the straight line ds, perpendicular to the projection of the meridian Pst. Remember that we want to find a point R such that we can descend to Ralong the great circle from S, and then to T along the great circle from R. We are going to search for R using the tangent plane, because R will be the summit of its great circle if the projections of its meridian and the great circle from it are perpendicular. Thus we should search for a point r in ds such that the angle Prt is 90°; in this way RT will be an arc of the great circle from R, because its projection rt will be perpendicular at r to the projection Pr of the meridian through R. To find the point r it is sufficient to recall a statement of elementary geometry: An inscribed angle spanning a semicircumference is 90°. Therefore



Figure 15.23: The projection of the great circle from $S(D_S)$ is the straight line ds, perpendicular to the projection of its meridian (the straight line Pst)

we draw the semicircumference whose diameter is the segment Pt (see Fig.15.24 below); the point where it intersects ds is the point r for which we were looking.



Figure 15.24: r is intersection of semicircumference(diameter = segment Pt) with line d_s

Next we find the point R in the sphere surface whose projection is r. In Fig. 15.25 below we see the spatial construction that enables us to find the point R, and the arcs of the great circle descents D_S and D_R that we travel on to reach T from S.



Figure 15.25: Join r with center of sphere and find R on spherical surface

We have already looked at the case in which the two points that we want to join using great circle descents are on the same meridian. Next, we examine the procedure used when the two points are on different meridians. In particular, we will examine the case when the two points are almost antipodes-points whose geographic longitudes differ by 180° .

Let us suppose that we intend to descend from the point S to another one on a lower latitude, which is on the other side (that is, 180° away) on the same meridian. First we project the point S onto the plane tangent to the sphere at the north pole (see Fig. 15.26 below).



Figure 15.26: Project point S onto plane tangent to sphere at North pole

Next, we divide the angle of 180° that separates the points of interest in the projection plane into, for example, eight parts. We start at s and make the construction in Fig. 15.27 below.



Figure 15.27: Going to the other side of the meridian

We call T the point on the sphere surface whose projection onto the plane is exactly the point t. The points S and T become linked by the arcs of great circle descents corresponding to the projections perpendicular to the lines dividing the 180° angle. (If we divide the 180° into smaller equal angles and make the previous construction, we could get from S to latitudes lower but almost equal to that of S). To find the spherical surface points we join each of the dividing points with the sphere's center (see Fig.15.28 below).



Figure 15.28: Project back to find the summits of the great circle descents

The points S and T are thus linked by the arcs of the succession of great circle descents shown in Fig. 15.29 below.



Figure 15.29: Find the arcs of the great circle descents

As we have mentioned, if we increase the divisions of the 180° angle, we will reach latitudes as close as we wish to that of the starting point. The connection with southerly points could be achieved either by varying one of the angles or following the method we have used before to join two points on the same meridian. In any case it is clear that we can always reach, starting from one point A of the northern hemisphere, any more southerly point than A (even if it is on the other side on the same meridian) by a finite sequence of great circle descents.

15.5.4 The Theorem

Using this lemma, we can determine if it is possible to assign values 0 or 1 to the points of the spherical surface so that we have exactly one 1 in each orthogonal triple. First let us see which distribution of zeros and ones the lemma implies. Let us begin with an orthogonal triple and assign 1 to one of the points and 0 to the other two. Let us place the 1 at the North Pole to facilitate the picture; all the points on the equator will thus take on the value 0 (see the proposition). Let us now consider the triple in Fig.15.30, where the great circle's plane forms an angle of more than 45° with the equator.



Figure 15.30: Great circle A forms an angle of more than 45° with the equator

If A has value 0, because A_E is on the equator and is therefore 0-valued, the point A_P would take on the value 1; consequently, all the points of the great circle descent from A would be 0-valued as well. But the latitude of A_P is less than 45°, which means that A_P is more southerly than A; thus we can reach A_P along a sequence of great circle descents from A. Because we can reason similarly about each one of these great circle descents, we ultimately conclude that A_P is 0-valued. (If the most northerly point of a great circle, say B, takes on the value 0, because B_E is on the equator and there- fore is 0-valued, B_P would take on the value 1. Therefore all the points of the great circle descent from B would also take on the value 0). We thus arrive at a contradiction and conclude that in a 45° dome around the north pole, all the points are 1-valued.

If all the points on the spherical surface within 45° of a 1-valued point have to take the value 1, then the points on the great circles perpendicular to those projectors-which occupy the central zone of the spherical surface-have to take on the value 0. In short, from the hypothesis that the projectors have welldefined values, we have reached the conclusion that the spherical surface must be distributed according to Fig.15.31 below: If we choose as the North Pole the direction of the original 1-valued projector, the points in the 45° domes around the North Pole and around the South Pole are 1-valued. The remaining points of the spherical surface are 0-valued.



Figure 15.31: Distribution of ones and zeros on the spherical surface

But the spherical surface's division into 1's and 0's that we have concluded is contradictory (in addition to clashing with quantum mechanics, that is, for quantum mechanics, and contrary to the result we have obtained, there is a nonzero probability that a projector within the upper skullcap takes on the value zero). Indeed, from the hypothesis that projectors have well-defined values, we have proven that if a projector is 1-valued, it has to be surrounded by a 45° dome made up of 1's. But let us look at a projector that forms, for example, 40° with the North Pole (P_{40} in Fig. 15.31). It also has the value 1; therefore all the projectors until P_{85} (a projector that forms 85° with the North Pole) should be 1-valued as well. But we had concluded that P_{85} was 0-valued. Consequently, we arrive at a contradiction. Thus it is impossible to distribute 1's and 0's on a spherical surface with the required condition. (In terms of color we see that if 1 means red and 0 means green and in each orthogonal triple there must be only one red point, it is impossible to color the spherical surface with these two colors). We have proven the KSB no-go theorem: It is impossible to ascribe values 0 or 1 to each point on a spherical surface so that we have exactly one 1 in each orthogonal triple.

We conclude that we cannot maintain a picture of a completely determinate world. We cannot think that reality exists out there, without observing it. Einstein was not happy with this state of affairs. He thought that there should be an objective world having definite properties whether or not they were measured. It was Pais who said that during a walk with him Einstein suddenly stopped, turned to Pais, and asked him whether he really believed that the moon existed only when one looked at it. The theorem we have just proved shows that the properties of microscopic systems are not completely defined before we look at them. The value of the projectors remains indefinite until we measure them. We need to accept a radically random world. The microscopic universe is blurred until we make an experiment and force it to choose one option. For this reason Peres has said that *unperformed experiments have no results*, preventing us from using counterfactual arguments.

Therefore, we have to admit that there are some commeasurable or co-decidable (simultaneously decidable) projectors and others that are not. Hence, there are some quantities that we can measure at the same time, but whose measuring excludes measuring other quantities that are not compatible with them. And we cannot say anything about the latter. The crux of the KSB theorem is that we cannot assign any value at all to them.

One of the authors of the theorem, Specker, related this problem to a question about the different kinds of God's knowledge of reality. In particular, the KSB theorem is related to the *future contingencies* of the philosopher and Jesuit Pedro Fonseca (1528-1599): those future events whose occurrence depends on an action taken by a creature exercising free will. According to Fonseca, God knows the outcome of unperformed experiments, or as he puts it, he knows what would happen if He put the will of the creatures in circumstances different from those in which He put them. Father Fonseca calls this knowledge middle science. But the KSB theorem proves that God does not have middle science. He cannot know what would happen if something different from what actually happens were to happen, that is, if a different projector had been measured.

15.5.5 The Discrete Version

Kochen and Specker's original paper did not deal with a continuous set of projectors. They searched for a finite number of projectors or directions leading to a contradiction like the one we have found. They arrived at a contradiction with a set of 117 directions. In 1990 Peres reduced that number to only 33. In 1991 Penrose heard Peres lecture on this work, and realized that Peres' directions matched those of a geometrical figure he had seen in a lithograph, *The Waterfall*, of the Dutch painter Escher (see the cap on the left tower of Fig. 15.32 below).



Figure 15.32: The left-hand tower has the quantum polyhedron

The figure is a polyhedron which is composed of three interpenetrating cubes, each obtained from the others by 90° rotations about lines joining the midpoints of its opposite edges (see Fig. 15.33 below).



Figure 15.33: The quantum polyhedron is made o three interpenetrating cubes

The 33 directions of Peres are the lines through opposite vertices, opposite edge

midpoints, and opposite face midpoints of each cube.

In Figs.15.34-15.39, each letter corresponds to the straight line going through the center of the cubes and the point closer to that letter. The straight lines going through the center of a face are designated as A_S (upper), A_L (lateral), and A_F (frontal) for the cube A, B_S , B_L , and B_F for the cube B, and C_S , C_L , and C_F for the cube C. The polyhedron's symmetry allows the following operations.



Figure 15.34: The directions on the cube ${\cal A}$



Figure 15.35: The directions on the two interpenetrating cubes A and B



Figure 15.36: The interpenetrating cubes A and B in perspective



Figure 15.37: The directions on the two interpenetrating cubes ${\cal A}$ and ${\cal C}$



Figure 15.38: The interpenetrating cubes A and C in perspective



Figure 15.39: The directions on the cube C

In the orthogonal triple A_SXY , we choose as the A_S direction the one with the value 1 so that the directions X and Y will take on the value 0. The directions A_L and A_F are 0-valued too, because they are perpendicular to A_S . In the triple B_SB_FY , the direction Y is 0-valued. From the two others, we choose B_S as the one with the value 1. In the triple C_SC_LX , the X is 0-valued. From the two others, we choose C_S as the one with the value 1. In the triple DEA_F , A_F is 0-valued. We can still choose the value of the two others. We choose D as the one with the value 1. The directions F and G are perpendicular to D as well; so they will take on the value 0.

In the triple HFY, H has the value 1, because F and Y are 0-valued. J takes on the value 0 because it is perpendicular to H. (It is clear that H and F are perpendicular because F becomes H when we turn the cube A 90° around Y, to generate the cube C).

In the triple $KC_L J$, K takes on the value 1 because it is orthogonal to C_L and J, which are 0-valued. L takes on the value 0 because it is perpendicular to K. In the triple MYL, M takes on the value 1 because it is orthogonal to Y and L. N takes on the value 0 because it is perpendicular to M. In the triple OA_LN , O takes on the value 1 because it is orthogonal to A_L and N. P takes on the value 0 because it is orthogonal to A_L and N. P takes on the value 0 because it is orthogonal to A_L and N. P takes on the value 0 because it is perpendicular to O. In QXP, Q takes on the value 1 because it is orthogonal to X and P. R takes on the value 0 because it is perpendicular to Q. In SB_FR , S takes on the value 1 because it is orthogonal to B_F and R, which are 0-valued. T takes on the value 0 because it is orthogonal to S. Finally, in XGT, X takes on the value 1 because it is orthogonal to G and T, which had the value 0. But X was 0-valued! Thus we arrive at a contradiction.

By using only a finite number of directions, we have shown again that it is not possible to assign 0,1 values to every direction if the condition that there is only one 1-valued direction for each orthogonal triple of directions is fulfilled. So we have again proved the KSB theorem.

How far does this theorem lead us? If, as shown, projectors and quantum observable quantities are not completely determined, we have a picture of microscopic reality with indefinite and ambiguous properties. Physical properties do not have, in general, objective existence independent of the act of observation. We should accept what Jordan had already said in 1934: Observations not only disturb what has to be measured, they produce it! In a measurement of position, for example, the electron is forced to a decision. We compel it to assume a definite position; previously it was, in general, neither here nor there; it had not yet made its decision for a definite position.... And Jordan concluded: We ourselves produce the results of measurement. The KSB theorem proves that we do not have an alternative picture of the subatomic world. That is its importance.

15.6 Problems

15.6.1 Measurements in a Stern-Gerlach Apparatus

(a) A spin-1/2 particle in the state $|S_z+\rangle$ goes through a Stern-Gerlach analyzer having orientation $\hat{n} = \cos \theta \hat{z} - \sin \theta \hat{x}$ (see figure below).



Figure 15.40: Tilted Stern-Gerlach Setup

What is the probability of finding the outgoing particle in the state?

(b) Now consider a Stern-Gerlach device of variable orientation as in the figure below.



Figure 15.41: Variable Orientation Stern-Gerlach Setup

More specifically, assume that it can have the three different directions

$$\hat{n}_1 = \hat{n} = \cos \theta \hat{z} - \sin \theta \hat{x}$$
$$\hat{n}_2 = \cos \left(\theta + \frac{2}{3}\pi\right) \hat{z} - \sin \left(\theta + \frac{2}{3}\pi\right) \hat{x}$$
$$\hat{n}_3 = \cos \left(\theta + \frac{4}{3}\pi\right) \hat{z} - \sin \left(\theta + \frac{4}{3}\pi\right) \hat{x}$$

with equal probability 1/3. If a particle in the state $|S_z+\rangle$ enters the analyzer, what is the probability that it will come out with spin eigenvalue $+\hbar/2$?

- (c) Calculate the same probability as above but now for a Stern-Gerlach analyzer that can have any orientation with equal probability.
- (d) A pair of particles is emitted with the particles in opposite directions in a singlet state |0,0⟩. Each particle goes through a Stern-Gerlach analyzer of the type introduced in (c); see figure below. Calculate the probability of finding the exiting particles with opposite spin eigenvalues.



Figure 15.42: EPR Stern-Gerlach Setup

15.6.2 Measurement in 2-Particle State

A pair of particles moving in one dimension is in a state characterized by the wave function

$$\psi(x_1, x_2) = N \exp\left[-\frac{1}{2\alpha}(x_1 - x_2 + a)^2\right] \exp\left[-\frac{1}{2\beta}(x_1 + x_2)^2\right]$$

- (a) Discuss the behavior of $\psi(x_1, x_2)$ in the limit $a \to 0$.
- (b) Calculate the momentum space wave function and discuss its properties in the above limit.
- (c) Consider a simultaneous measurement of the positions x_1 and x_2 of the two particles when the system is in the above state. What are the expected position values? What are the values resulting from simultaneous measurement of the momenta p_1 and p_2 of the two particles?

15.6.3 Measurements on a 2 Spin-1/2 System

(a) Consider a system of two spin-1/2 particles in the singlet state

$$|1,0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{(1)} |\downarrow\rangle_{(2)} - |\downarrow\rangle_{(1)} |\uparrow\rangle_{(2)} \right)$$

and perform a measurement of $S_z^{(1)}$. Comment on the fact that a simultaneous measurement of $S_z^{(2)}$ gives an outcome that can always be predicted form the first-mentioned measurement. Show that this property, entanglement, is not shared by states that are tensor products. Is this state

$$|\psi\rangle = \frac{1}{2} \left(|1,1\rangle + \sqrt{2} |1,0\rangle + |1,-1\rangle \right)$$

entangled, i.e., is it a tensor product?

(b) Consider now the set of four states $|a\rangle$, a = 0, 1, 2, 3:

$$\begin{aligned} |0\rangle &= \frac{1}{\sqrt{2}} \left(|1,1\rangle + i |1,-1\rangle \right) \\ |1\rangle &= \frac{1}{\sqrt{2}} \left(|1,-1\rangle + i |1,1\rangle \right) \\ |2\rangle &= \frac{1}{\sqrt{2}} \left(e^{-i\pi/4} |1,0\rangle - e^{i\pi/4} |0,0\rangle \right) \\ |3\rangle &= \frac{1}{\sqrt{2}} \left(e^{-i\pi/4} |1,0\rangle + e^{i\pi/4} |0,0\rangle \right) \end{aligned}$$

Show that these states are entangled and find the unitary matrix $U_{a\alpha}$ such that

$$|a\rangle = U_{a\alpha} |\alpha\rangle$$

where $\{ |\alpha \rangle \} = |1,1\rangle, |1,-1\rangle, |1,0\rangle, |0,0\rangle.$

(c) Consider a one-particle state $|\psi\rangle = C_+ |\uparrow\rangle + C_- |\downarrow\rangle$ and one of the entangled states considered in (b), for example $|0\rangle$. Show that the product state can be written as

$$|\psi\rangle|0\rangle = \frac{1}{2} (|0\rangle|\psi\rangle + |1\rangle|\psi'\rangle + |2\rangle|\psi''\rangle + |3\rangle|\psi'''\rangle)$$

where the states $|\psi'\rangle$, $|\psi''\rangle$, $|\psi''\rangle$, are related to $|\psi\rangle$ through a unitary transformation

15.6.4 Measurement of a Spin-1/2 Particle

A spin-1/2 electron is sent through a solenoid with a uniform magnetic field in the y direction and then measured with a Stern-Gerlach apparatus with field gradient in the x direction as shown below:



Figure 15.43: EPR Stern-Gerlach Setup

The time spent inside the solenoid is such that $\Omega t = \varphi$, where $\Omega = 2\mu_B B/\hbar$ is the Larmor precession frequency.

(a) Suppose the input state is the pure state $|\uparrow_z\rangle$. Show that the probability for detector D_A to fire as a function of φ is

$$P_{D_A} = \frac{1}{2} \left(\cos(\varphi/2) + \sin(\varphi/2) \right)^2 = \frac{1}{2} \left(1 + \sin\varphi \right)$$

Repeat for the state $|\downarrow_z\rangle$ and show that

$$P_{D_A} = \frac{1}{2} \left(\cos(\varphi/2) - \sin(\varphi/2) \right)^2 = \frac{1}{2} \left(1 - \sin\varphi \right)$$

(b) Now suppose the input is a pure coherent superposition of these two states,

$$\left|\uparrow_{x}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow_{z}\right\rangle + \left|\downarrow_{z}\right\rangle\right)$$

Find and sketch the probability for detector D_A to fire as a function of φ .

(c) Now suppose the input state is the completely mixed state

$$\hat{\rho} = \frac{1}{2} \left(\left| \uparrow_z \right\rangle \left\langle \uparrow_z \right| + \left| \downarrow_z \right\rangle \left\langle \downarrow_z \right| \right)$$

Find and sketch the probability for detector D_A to fire as a function of φ . Comment on the result.

15.6.5 Mixed States vs. Pure States and Interference

A *spin-interferometer* is shown below:

Spin-1/2 electrons prepared in a given state (pure or mixed) are separated into two paths by a Stern-Gerlach apparatus (gradient field along z). In one path,



Figure 15.44: Spin-Interferometer Setup

the particle passes through a solenoid, with a uniform magnetic field along the x-axis. The two paths are then recombined, sent through another Stern-Gerlach apparatus with field gradient along x, and the particles are counted in detectors in the two emerging ports.

The strength of the magnetic field is chosen so that $\Omega t = \varphi$, for some phase φ , where $\Omega = 2\mu_B B/\hbar$ is the Larmor frequency and t is the time spent inside the solenoid.

(a) Derive the probability of electrons arriving at detector D_A as a function of φ for the following pure state inputs:

(i)
$$|\uparrow_z\rangle$$
 , (ii) $|\downarrow_z\rangle$, (iii) $|\uparrow_x\rangle$, (iv) $|\downarrow_x\rangle$

Comment on your results.

(b) Remember that for a mixed state we have

$$\hat{\rho} = \sum_{i} p_{i} \left| \psi_{i} \right\rangle \left\langle \psi_{i} \right|$$

where p_i is the probability of $|\psi_i\rangle$.

This is a statistical mixture of the states $\{|\psi_i\rangle\}$, not a coherent superposition of states. We should think of it *classically*, i.e., we have one of the set $\{|\psi_i\rangle\}$, we just do not know which one.

Prove that

$$P_{D_{A}} = Tr\left[\left|\uparrow_{x}\right\rangle\left\langle\uparrow_{x}\right|\hat{\rho}\right] = \sum_{i} p_{i}\left|\left\langle\uparrow_{x}\right|\psi_{i}\right\rangle\right|^{2}$$

where $|\langle \uparrow_x | \psi_i \rangle|^2$ = the probability of detector B firing for the given input state (we figured these out in part (a)). Repeat part (a) for the following mixed state inputs:

$$\begin{array}{l} (i) \quad \hat{\rho} = \frac{1}{2} \left| \uparrow_z \right\rangle \left\langle \uparrow_z \right| + \frac{1}{2} \left| \downarrow_z \right\rangle \left\langle \downarrow_z \right| & , \quad (ii) \quad \hat{\rho} = \frac{1}{2} \left| \uparrow_x \right\rangle \left\langle \uparrow_x \right| + \frac{1}{2} \left| \downarrow_x \right\rangle \left\langle \downarrow_x \right| & , \\ (iii) \quad \hat{\rho} = \frac{1}{3} \left| \uparrow_z \right\rangle \left\langle \uparrow_z \right| + \frac{2}{3} \left| \downarrow_z \right\rangle \left\langle \downarrow_z \right| & , \end{array}$$

15.6.6 Which-path information, Entanglement, and Decoherence

If we can determine which path a particle takes in an interferometer, then we do not observe quantum interference fringes. But how does this arise?

Consider the interferometer shown below:



Figure 15.45: Spin-Interferometer Setup

Into one arm of the interferometer we place a which-way detector in the form of another spin-1/2 particle prepared in the state $|\uparrow_z\rangle_W$. If the electron which travels through the interferometer, and is ultimately detected (denoted by subscript D), interacts with the which-way detector, the which-way electron flips the spin $|\uparrow_z\rangle_W \rightarrow |\downarrow_z\rangle_W$, i.e, the "which-way" detector works such that

If
$$|\psi\rangle_D = |\uparrow_z\rangle_D$$
 nothing happens to $|\uparrow_z\rangle_W$

If
$$|\psi\rangle_D = |\downarrow_z\rangle_D$$
, then $|\uparrow_z\rangle_W \to |\downarrow_z\rangle_W$ (a spin flip)

Thus, as a composite system

$$|\uparrow_{z}\rangle_{D}|\uparrow_{z}\rangle_{W} \to |\uparrow_{z}\rangle_{D}|\uparrow_{z}\rangle_{W} \qquad |\downarrow_{z}\rangle_{D}|\uparrow_{z}\rangle_{W} \to |\uparrow_{z}\rangle_{D}|\downarrow_{z}\rangle_{W}$$
(15.339)

(a) The electron D is initially prepared in the state $|\uparrow_x\rangle_D = (|\uparrow_z\rangle_D + |\downarrow_z\rangle_D)/\sqrt{2}$. Show that before detection, the two electrons D and W are in an entangled state

$$|\Psi_{DW}\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow_z\rangle_D |\uparrow_z\rangle_W + |\downarrow_z\rangle_D |\downarrow_z\rangle_W\right)$$

(b) Only the electron D is detected. Show that its *marginal state*, ignoring the electron W, is the completely mixed state,

$$\hat{\rho}_{D} = \frac{1}{2} \left| \uparrow_{z} \right\rangle_{D D} \left\langle \uparrow_{z} \right| + \frac{1}{2} \left| \downarrow_{z} \right\rangle_{D D} \left\langle \downarrow_{z} \right|$$

This can be done by calculating

$$\operatorname{Prob}(m_D) = \sum_{m_W} |\langle m_D, m_W | \Psi_{DW} \rangle|^2$$

for some observable.

This state shows no interference between $|\uparrow_z\rangle_D$ and $|\downarrow_z\rangle_D$. Thus, the emphwhich-way detector removes the coherence between states that existed in the input.

(c) Suppose now the which-way detector does not function perfectly and does not completely flip the spin, but rotates it by an angle θ about x so that

 $|\uparrow_{\theta}\rangle_{W} = \cos(\theta/2) |\uparrow_{z}\rangle_{W} + \sin(\theta/2) |\downarrow_{z}\rangle_{W}$

Show that in this case the marginal state is

$$\hat{\rho}_{D} = \frac{1}{2} |\uparrow_{z}\rangle_{D D} \langle\uparrow_{z}| + \frac{1}{2} |\downarrow_{z}\rangle_{D D} \langle\downarrow_{z}| + \cos(\theta/2) |\uparrow_{z}\rangle_{D D} \langle\downarrow_{z}| + \sin(\theta/2) |\downarrow_{z}\rangle_{D D} \langle\uparrow_{z}|$$

Comment on the limits $\theta \to 0$ and $\theta \to \pi$.

15.6.7 Livio and Oivil

Two scientists (they happen to be twins, named *Oivil* and *Livio*, but never mind) decide to do the following experiment. They set up a light source, which emits two photons at a time, back-to-back in the laboratory frame. The ensemble is given by

$$\rho = \frac{1}{2} \left(\left| LL \right\rangle \left\langle LL \right| + \left| RR \right\rangle \left\langle RR \right| \right)$$

where L refers to left-handed polarization and R refers to right-handed polarization. Thus, $|LR\rangle$ would refer to the state in which photon number 1 (defined as the photon which is aimed at Oivil, say) is left-handed and photon number 2 (the photon aimed at scientist Livio) is right-handed.

These scientists (one of whom has a diabolical bent) decide to play a game with Nature: Oivil (of course) stays in the lab, while Livio treks to a point a lightyear away. The light source is turned on and emits two photons, one directed toward each scientist. Oivil soon measures the polarization of his photon; it is left-handed. He quickly makes a note that his sister is going to see a left-handed photon, about a year from that time.

The year has passed and finally Livio sees her photon, and measures its polarization. She sends a message back to her brother Oivil, who learns in yet another year what he know all along; Livio's photon was left-handed.

Oivil then has a sneaky idea. He secretly changes the apparatus, without telling his forlorn sister. Now the ensemble is

$$\rho = \frac{1}{2} \left(|LL\rangle + |RR\rangle \right) \left(\left\langle LL | + \left\langle RR | \right\rangle \right)$$

He causes another pair of photons to be emitted with this new apparatus and repeats the experiment. The result is identical to the first experiment.

- (a) Was Oivil lucky, or will he get the right answer every time, for each apparatus? Demonstrate the answer explicitly using the density matrix formalism.
- (b) What is the probability that Livio will observe a left-handed photon, or a right-handed photon, for each apparatus? Is there a problem with causality here? How can Oivil know what Livio is going to see, long before she sees it? Discuss what is happening here. Feel free to modify the experiment to illustrate any points you wish to make.

15.6.8 Measurements on Qubits

You are given one of two quantum states of a single qubit(physical system representing a 2-valued state): either $|\phi\rangle = |0\rangle$ or $|\phi\rangle = \cos \theta |0\rangle + \sin \theta |1\rangle$. You want to make a single measurement that best distinguishes between these two states, i.e., you want to find the best basis for making a measurement to distinguish the two states. So let us measure the qubit in the basis $\{|\nu\rangle = \alpha |0\rangle + \beta |1\rangle, |\nu^{\perp}\rangle\}$, where α, β are to be determined for optimal success. For outcome $|\nu\rangle$ we guess that the qubit was in state $|0\rangle$; for outcome $|\nu^{\perp}\rangle$ we guess that the qubit was in state $|0\rangle$; for outcome $|\nu^{\perp}\rangle$ we guess that the qubit was in state $|\phi\rangle$. Determine the optimal measurement basis given this procedure. You can take α and β to be real numbers, in which case the normalization $|\alpha|^2 + |\beta|^2 = 1$ implies that you can write α and β as, e.g. $\alpha = \sin \gamma$ and $\beta = \cos \gamma$. HINT: you will need to first construct the probability of a correct measurement in this situation. You should convince yourselves that this is given by

 $Pr[qubit was |0\rangle] Pr[|\nu\rangle| qubit was |0\rangle] + Pr[qubit was |\psi\rangle] Pr[|\nu^{\perp}\rangle| qubit was |\psi\rangle]$

where, e.g.

$$Pr[|\nu\rangle | qubit was |0\rangle] = |\langle \nu | 0\rangle|^2$$

If the state you are presented with is either $|\phi\rangle$ or $|\psi\rangle$ with 50% probability each, what is the probability that your measurement correctly identifies the state?

15.6.9 To be entangled....

Let $\mathcal{H}_A = span\{|0_A\rangle, |1_A\rangle\}$ and $\mathcal{H}_B = span\{|0_B\rangle, |1_B\rangle\}$ be two-dimensional Hilbert spaces and let $|\Psi_{AB}\rangle$ be a factorizable state in the joint space $\mathcal{H}_A \otimes \mathcal{H}_B$. Specify necessary and sufficient conditions on $|\Psi_{AB}\rangle$ such that $U_{AB} |\Psi_{AB}\rangle$ is an entangled state where

$$U_{AB} = |0_A\rangle \langle 0_A| \otimes |0_B\rangle \langle 0_B| - |1_A\rangle \langle 1_A| \otimes |1_B\rangle \langle 1_B|$$

15.6.10 Alice, Bob and Charlie

Let Alice, Bob and Charlie be in possession of quantum systems whose states live in $\mathcal{H}_A = span\{|0_A\rangle, |1_A\rangle\}, \mathcal{H}_B = span\{|0_B\rangle, |1_B\rangle\}$ and $\mathcal{H}_C = span\{|0_C\rangle, |1_C\rangle\},$ respectively. Suppose that a joint state of these systems has been prepared as the (three-way) entangled state

$$|\Psi_{ABC}\rangle = \frac{1}{\sqrt{2}} \left(|0_A 0_B 0_C\rangle + |1_A 1_B 1_C\rangle \right)$$

- (a) What is the reduced density operator on $\mathcal{H}_A \otimes \mathcal{H}_B$ if we take a partial trace over \mathcal{H}_C ?
- (b) Suppose Charlie performs a measurement specified by the partial projectors $1^A \otimes 1^B \otimes |0_C\rangle \langle 0_C|$ and $1^A \otimes 1^B \otimes |1_C\rangle \langle 1_C|$. Compute the probabilities of the possible outcomes, as well as the corresponding post-measurement states. Show that this ensemble is consistent with your answer to part (a)
- (c) Suppose Charlie performs a measurement specified by the partial projectors $1^A \otimes 1^B \otimes |x_C\rangle \langle x_C|$ and $1^A \otimes 1^B \otimes |y_C\rangle \langle y_C|$, where

$$|x_C\rangle = \frac{1}{\sqrt{2}} \left(|0_C\rangle + |1_C\rangle \right) \quad , \quad |y_C\rangle = \frac{1}{\sqrt{2}} \left(|0_C\rangle - |1_C\rangle \right)$$

Again, compute the probabilities of the possible outcomes and the corresponding post-measurement states and show that this ensemble is consistent with your answer from part (a).

(d) Suppose Alice and Bob know that Charlie has performed one of the two measurements from parts (b) and (c), but they do not know which (assume equal probabilities) measurement he performed nor do they know the outcome. Write down the quantum ensemble that you think Alice and Bob should use to describe the post-measurement state on $\mathcal{H}_A \otimes \mathcal{H}_B$. Is this consistent with the reduced density operator from part (a)? How should Alice and Bob change their description of the post-measurement state if Charlie subsequently tells them which measurement he performed and what the outcome was?

Chapter 16

The EPR Argument and Bell Inequality

16.1 Hidden variables and Bell's Inequalities-1st Try

As we have seen, when a quantum system possesses more than one degree of freedom, the associated Hilbert space is a tensor product of the spaces associated with each degree of freedom. This structure leads to specific properties of quantum mechanics, whose *paradoxical* nature has been discussed in earlier chapters. In this section we will study an example of such a situation by considering entangled states for the spins of two particles.

The system under consideration is a hydrogen atom which is dissociated into an electron and a proton. We consider the spin states of these two particles when they have left the dissociation region and are located in spatially distinct regions, e.g. a few meters from one another. They are then considered to be free particles whose spin states do not evolve.

16.1.1 The Electron Spin

Consider a unit vector \hat{u}_{ϕ} n the (z, x) plane given by $\hat{u}_{\phi} = \cos \phi \hat{u}_z + \sin \phi \hat{u}_x$ where \hat{u}_x and \hat{u}_z are unit vectors in the x and z directions. We note that $\hat{S}_{e\phi} = \hat{S}_e \cdot \hat{u}_{\phi}$ is the component of the electron spin in the \hat{u}_{ϕ} direction.

In the eigenbasis $|e:\pm\rangle$ of \hat{S}_{ez} , the matrix representing $\hat{S}_{e\phi}$ is

$$\begin{pmatrix} \langle +|\hat{S}_{e\phi}|+\rangle & \langle +|\hat{S}_{e\phi}|-\rangle \\ \langle -|\hat{S}_{e\phi}|+\rangle & \langle -|\hat{S}_{e\phi}|-\rangle \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \cos\phi & \sin\phi \\ \sin\phi & -\cos\phi \end{pmatrix}$$
(16.1)

which has eigenvalues $\pm \hbar/2$ (true for any direction).

The corresponding eigenvectors are

$$|e:+\phi\rangle = \cos\frac{\phi}{2}|e:+\rangle + \sin\frac{\phi}{2}|e:-\rangle \tag{16.2}$$

$$|e:-\phi\rangle = -\sin\frac{\phi}{2}|e:+\rangle + \cos\frac{\phi}{2}|e:-\rangle \tag{16.3}$$

If the electron is emitted in the state $|e:+\phi\rangle$, the probability $P_+(\alpha)$ of finding the electron in the state $|e:+\alpha\rangle$ is given by

$$P_{+}(\alpha) = |\langle e:+\alpha \mid e:+\phi \rangle|^{2}$$

$$= \left| \left(\cos \frac{\alpha}{2} \langle e:+| + \sin \frac{\alpha}{2} \langle e:-| \right) \left(\cos \frac{\phi}{2} \mid e:+\rangle + \sin \frac{\phi}{2} \mid e:-\rangle \right) \right|^{2}$$

$$= \left| \left(\cos \frac{\alpha}{2} \cos \frac{\phi}{2} + \sin \frac{\alpha}{2} \sin \frac{\phi}{2} \right) \right|^{2} = \cos^{2} \frac{\phi - \alpha}{2}$$
(16.4)

and similarly,

$$P_{-}(\alpha) = \left| \left\langle e : -\alpha \mid e : +\phi \right\rangle \right|^{2}$$
$$= \left| \left(-\sin\frac{\alpha}{2} \left\langle e : +\right| + \cos\frac{\alpha}{2} \left\langle e : -\right| \right) \left(\cos\frac{\phi}{2} \mid e : +\rangle + \sin\frac{\phi}{2} \mid e : -\rangle \right) \right|^{2}$$
$$= \left| \left(-\sin\frac{\alpha}{2}\cos\frac{\phi}{2} + \cos\frac{\alpha}{2}\sin\frac{\phi}{2} \right) \right|^{2} = \sin^{2}\frac{\phi - \alpha}{2}$$
(16.5)

Using these results, the expectation value of $\hat{S}_{e\alpha}$ in the $|e:+\phi\rangle$ state is then

16.1.2 Correlations Between the Two Spins

We assume that after the dissociation, the electron-proton system is in the factorized spin state $|e:+\phi\rangle \otimes |p:-\phi\rangle$. Now if $|u_1\rangle \in E$ and $|u_2\rangle \in E$ and $|v_1\rangle \in F$ and $|v_2\rangle \in F$, then $|u\rangle \otimes |v\rangle \in G = E \otimes F$ and if \hat{A} and \hat{B} act respectively in E and F, then $\hat{C} = \hat{A} \otimes \hat{B}$ acts in G. Then one has $\langle u_2 | \otimes \langle v_2 | \hat{C} | u_1 \rangle \otimes |v_1\rangle = \langle u_2 | \hat{A} | u_1 \rangle \langle v_2 | \hat{B} | v_1 \rangle$.

We now determine the probability $P_+(\alpha)$ of finding $+\hbar/2$ when measuring the component $\hat{S}_{e\alpha}$ of the electron spin in this state.

The projector on the eigenstate $|e:+\alpha\rangle$, corresponding to the measured value, is $|e:+\alpha\rangle\langle e:+\alpha|\otimes \hat{I}_p$, where \hat{I}_p is the identity operator on the proton states.

Therefore,

$$P_{+}(\alpha) = \langle p : -\phi | \otimes \langle e : +\phi | (|e : +\alpha) \langle e : +\alpha | \otimes \hat{I}_{p}) | e : +\phi \rangle \otimes |p : -\phi \rangle$$
$$= \langle p : -\phi | \hat{I}_{p} | p : -\phi \rangle \langle e : +\phi | e : +\alpha \rangle \langle e : +\alpha | e : +\phi \rangle$$
$$= |\langle e : +\alpha | e : +\phi \rangle|^{2} = \cos^{2} \frac{\phi - \alpha}{2}$$
(16.7)

and the state after the measurement is $|e:+\alpha\rangle \otimes |p:-\phi\rangle$. The proton spin is not affected, because the initial state is factorized (and all probability laws are factorized).

For $\hat{u}_{\phi} = \cos \phi \hat{u}_z + \sin \phi \hat{u}_x$ and $\hat{u}_{\beta} = \cos \beta \hat{u}_z + \sin \beta \hat{u}_x$ we can calculate the expectation values (as earlier)

$$\langle \hat{S}_{e\alpha} \rangle = \frac{\hbar}{2} \cos(\phi - \alpha) \quad , \quad \langle \hat{S}_{p\beta} \rangle = -\frac{\hbar}{2} \cos(\phi - \beta)$$
 (16.8)

The correlation coefficient between the two spins $E(\alpha, \beta)$ is defined by

$$E(\alpha,\beta) = \frac{\left\langle \hat{S}_{e\alpha} \otimes \hat{S}_{p\beta} \right\rangle - \left\langle \hat{S}_{e\alpha} \right\rangle \left\langle \hat{S}_{p\beta} \right\rangle}{\left(\left\langle \hat{S}_{e\alpha}^2 \right\rangle \left\langle \hat{S}_{p\beta}^2 \right\rangle \right)^{1/2}}$$
(16.9)

Now

$$\hat{S}_{e\alpha}^2 = \frac{\hbar^2}{4}\hat{I}_e \quad , \quad \hat{S}_{p\beta}^2 = \frac{\hbar^2}{4}\hat{I}_p \tag{16.10}$$

and

$$\left\langle \hat{S}_{e\alpha} \otimes \hat{S}_{p\beta} \right\rangle = \left\langle e : +\alpha \right| \hat{S}_{e} \left| e : +\alpha \right\rangle \left\langle p : +\beta \right| \hat{S}_{p} \left| p : +\beta \right\rangle$$
$$= -\frac{\hbar^{2}}{4} \cos(\phi - \alpha) \cos(\phi - \beta)$$
(16.11)

Thus,

$$E(\alpha,\beta) = \frac{-\frac{\hbar^2}{4}\cos(\phi-\alpha)\cos(\phi-\beta) + \frac{\hbar^2}{4}\cos(\phi-\alpha)\cos(\phi-\beta)}{\frac{\hbar^2}{4}} = 0$$

This just reflects the fact that in a factorized state, the two spin variables are independent.

Correlations in the Singlet State

Now assume that, after the dissociation, the two particles are in the singlet spin state

$$|\psi_s\rangle = \frac{1}{\sqrt{2}} \left(|e:+\rangle \otimes |p:-\rangle - |e:-\rangle \otimes |p:+\rangle\right)$$
(16.12)

If we measure the component $\hat{S}_{e\alpha}$ of the electron spin along the direction $\hat{u}_{\alpha} = \cos \alpha \hat{u}_z + \sin \alpha \hat{u}_x$, we find the following results and corresponding probabilities: there are two possible values

$$\begin{aligned} & +\frac{\hbar}{2} \Leftrightarrow projector \quad |e:+\alpha\rangle \langle e:+\alpha| \otimes \hat{I}_p \\ & -\frac{\hbar}{2} \Leftrightarrow projector \quad |e:-\alpha\rangle \langle e:-\alpha| \otimes \hat{I}_p \end{aligned}$$

with probabilities

$$P_{+}(\alpha) = \left(|\langle e : +\alpha \mid e : + \rangle|^{2} + |\langle e : +\alpha \mid e : - \rangle|^{2} \right) = \frac{1}{2}$$
$$P_{-}(\alpha) = \left(|\langle e : -\alpha \mid e : + \rangle|^{2} + |\langle e : -\alpha \mid e : - \rangle|^{2} \right) = \frac{1}{2}$$

This result is a consequence of the rotational invariance of the singlet state.

Now suppose the result of this measurement is $+\hbar/2$ and then later on, one measures the component $\hat{S}_{p\beta}$ of the proton spin along the direction $\hat{u}_{\beta} = \cos\beta \hat{u}_z + \sin\beta \hat{u}_x$.

Since the electron spin is measured to be $+\hbar/2$, the state after that measurement is

$$\langle e:+\alpha \mid \psi_s \rangle \mid e:+\alpha \rangle = \frac{1}{\sqrt{2}} (\langle e:+\alpha \mid e:+\rangle \mid e:+\alpha \rangle \otimes \mid p:-\rangle - \langle e:+\alpha \mid e:-\rangle \mid e:+\alpha \rangle \otimes \mid p:+\rangle)$$

$$\Rightarrow \cos \frac{\alpha}{2} \mid e:+\alpha \rangle \otimes \mid p:-\rangle - \sin \frac{\alpha}{2} \mid e:+\alpha \rangle \otimes \mid p:+\rangle$$
(16.13)

The probabilities for the two possible results of measurement of the proton spin, $\pm \hbar/2$, are

$$P_{+}(\beta) = \sin^{2} \frac{\alpha - \beta}{2} , \quad P_{-}(\beta) = \cos^{2} \frac{\alpha - \beta}{2}$$
 (16.14)

What would have happened if we had measured the proton spin first?

If the proton had been measured first then we would have

$$P_{+}(\beta) = \frac{1}{2}$$
, $P_{-}(\beta) = \frac{1}{2}$ (16.15)

as we found for the electron when the electron was measured first.

The fact that the measurement on the electron affects the probabilities of the results of a measurement on the proton, although the two particles are spatially separated, is in contradiction to Einstein's assertion or belief that *the real states* of two spatially separated objects must be independent of one another. This is the starting point of the EPR paradox. Quantum mechanics is not a local theory as far as measurements are concerned.

Note, however, that this non-locality does not allow the instantaneous transmission of information, From a measurement of the proton spin, one can not determine whether the electron spin has been previously measured. It is only when, for a series of experiments, the results of the measurements on the electron and the proton are later compared, that one can find this non-local character of quantum mechanics.

We now recalculate the expectations values $\langle \hat{S}_{e\alpha} \rangle$ and $\langle \hat{S}_{p\beta} \rangle$ in the singlet state. We get (using the same process as above) $\langle \hat{S}_{e\alpha} \rangle = 0 = \langle \hat{S}_{p\beta} \rangle$. This is so because one does not worry about the other variable.

Finally, we can calculate the correlation coefficient in the singlet state. We have, since the spins are correlated now, that

$$\left\langle \hat{S}_{e\alpha} \otimes \hat{S}_{p\beta} \right\rangle = \frac{\hbar^2}{4} \left(\sin^2 \frac{\alpha - \beta}{2} - \cos^2 \frac{\alpha - \beta}{2} \right) = -\frac{\hbar^2}{4} \cos(\alpha - \beta) \tag{16.16}$$

and therefore

$$E(\alpha,\beta) = \frac{-\frac{\hbar^2}{4}\cos(\alpha-\beta) + 0}{\frac{\hbar^2}{4}} = -\cos(\alpha-\beta)$$
(16.17)

in the singlet state.

16.1.3 A Simple Hidden Variable Model

For Einstein and several other physicists, the solution to the *paradox* uncovered above comes from the fact that the states of quantum mechanics, in particular the singlet state above, provide and incomplete description of reality. A *complete* theory (for predicting spin measurements, in the present case) should incorporate additional variables or parameters, whose knowledge would render measurements independent for two spatially separated objects. However, present experiments cannot determine the values of these parameters, which are therefore called *hidden variables*. The experimental result should then consist of some averaging over these unknown parameters.

In the case of interest, a very simplified example of such a theory is the following. We assume that, after each dissociation, the system is in a factorized state $|e:+\phi\rangle \otimes |p:-\phi\rangle$, but that the direction ϕ varies from one event to another. In this case ϕ is the hidden variable. We assume that all directions of ϕ are equally probable, i.e., the probability density that the decay occurs with direction ϕ is uniform and equal to $1/2\pi$.

Since we are ignorant of the value of $\phi,$ the expectation value of an observable \hat{A} is now defined to be

$$\left\langle \hat{A} \right\rangle = \frac{1}{2\pi} \int_{0}^{2\pi} \left\langle e : +\phi \right| \otimes \left\langle p : -\phi \right| \hat{A} \left| e : +\phi \right\rangle \otimes \left| p : -\phi \right\rangle \tag{16.18}$$

Let us now use this new definition of the expectation value to investigate the correlation coefficient. We have from earlier

$$E(\alpha,\beta) = \frac{\left\langle \hat{S}_{e\alpha} \otimes \hat{S}_{p\beta} \right\rangle - \left\langle \hat{S}_{e\alpha} \right\rangle \left\langle \hat{S}_{p\beta} \right\rangle}{\left(\left\langle \hat{S}_{e\alpha}^2 \right\rangle \left\langle \hat{S}_{p\beta}^2 \right\rangle \right)^{1/2}}$$

Using our earlier results we have

$$\left\langle \hat{S}_{e\alpha} \right\rangle = \frac{\hbar^2}{4} \int \cos(\phi - \alpha) \frac{d\phi}{2\pi} = 0 \tag{16.19}$$

and similarly $\langle \hat{S}_{p\beta} \rangle = 0$. We also have

$$\left\langle \hat{S}_{e\alpha} \otimes \hat{S}_{p\beta} \right\rangle = -\frac{\hbar^2}{4} \int \cos(\phi - \alpha) \cos(\phi - \beta) \frac{d\phi}{2\pi} = -\frac{\hbar^2}{8} \cos(\alpha - \beta) \qquad (16.20)$$

Therefore, in this simple hidden variable model

$$E(\alpha,\beta) = -\frac{1}{2}\cos(\alpha - \beta)$$
(16.21)

In such a model, one finds a non-vanishing correlation coefficient, which is an interesting observation. Even more interesting is that the correlation is smaller than the prediction of quantum mechanics by a factor of 2.

The first precise experimental tests of hidden variable descriptions versus quantum mechanics have been performed on correlated pairs of photons emitted in an atomic cascade. Although, we are not dealing with pin-1/2 particles in this case (see discussion later in this chapter), the physical content is basically the same as in this case. As an example Figure 16.1 below presents the experimental results of Aspect, et al,



Figure 16.1: Data from Aspect, etal

It gives the variation of $E(\alpha, \beta)$ as a function of the difference $\alpha - \beta$, which is found experimentally to be the only relevant quantity, i.e., the results do not depend in any way on α or β separately! The circles indicate the size of experimental errors.

The experimental points agree with the predictions of quantum mechanics and clearly disagree, therefore, with the predictions of this particular hidden variables theory.
16.2 Bell's Theorem and Experimental Results

As proved by Bell in 1965, the disagreement between the predictions of quantum mechanics and those of hidden variable theories is actually very general when one considers correlation measurements on entangled states.

We can, however, show that the correlation results for hidden variable theories are constrained by what is known as Bell's inequality, which is violated by quantum mechanics.

Consider a hidden variable theory, whose results consists of two functions $A(\lambda, \hat{u}_{\alpha})$ and $B(\lambda, \hat{u}_{\beta})$ giving respectively the results of the electron and proton spin measurements. Each of these two functions takes only two values $+\hbar/2$ and $-\hbar/2$. It depends on the value of the hidden variable λ for the considered electron-proton pair. The nature of the hidden variable need not be further specified for this discussion. The result A of course depends on the axis \hat{u}_{α} chosen for the measurement of the electron spin, but it *does* not depend on the axis \hat{u}_{β} . Similarly B does not depend on \hat{u}_{α} . This *locality* hypothesis is essential for the following discussion.

Note that we assume here that the hidden variable theory reproduces the one operator averages found for the singlet state:

$$\langle \hat{S}_{e\alpha} \rangle = \int P(\lambda) A(\lambda, \hat{u}_{\alpha}) d\lambda = 0$$
 (16.22)

$$\langle \hat{S}_{p\beta} \rangle = \int P(\lambda)B(\lambda, \hat{u}_{\beta})d\lambda = 0$$
 (16.23)

If this was not the case, such a hidden variable theory should clearly be rejected since it would not reproduce a well-established experimental result.

Let us now consider the quantity

$$A(\lambda, \hat{u}_{\alpha})B(\lambda, \hat{u}_{\beta}) + A(\lambda, \hat{u}_{\alpha})B(\lambda, \hat{u}_{\beta}') + A(\lambda, \hat{u}_{\alpha}')B(\lambda, \hat{u}_{\beta}') - A(\lambda, \hat{u}_{\alpha}')B(\lambda, \hat{u}_{\beta})$$
(16.24)

for any set $\hat{u}_{\alpha}, \hat{u}_{\beta}, \hat{u}'_{\alpha}, \hat{u}'_{\beta}$. We can rewrite this as

$$A(\lambda, \hat{u}_{\alpha})(B(\lambda, \hat{u}_{\beta}) + B(\lambda, \hat{u}_{\beta}')) + A(\lambda, \hat{u}_{\alpha}')(B(\lambda, \hat{u}_{\beta}') - B(\lambda, \hat{u}_{\beta}))$$
(16.25)

Now the two quantities $B(\lambda, \hat{u}_{\beta})$ and $B(\lambda, \hat{u}_{\beta}')$ can take on only two values $\pm \hbar/2$. Therefore, one has either

$$B(\lambda, \hat{u}_{\beta}) + B(\lambda, \hat{u}_{\beta}') = \pm \hbar \quad , \quad B(\lambda, \hat{u}_{\beta}') - B(\lambda, \hat{u}_{\beta}) = 0 \tag{16.26}$$

or

$$B(\lambda, \hat{u}_{\beta}) + B(\lambda, \hat{u}_{\beta}') = 0 \quad , \quad B(\lambda, \hat{u}_{\beta}') - B(\lambda, \hat{u}_{\beta}) = \pm\hbar$$
(16.27)

Therefore, since $|A(\lambda, \hat{u}_{\alpha})| = |A(\lambda, \hat{u}'_{\alpha})| = \hbar/2$, we have the result

$$A(\lambda, \hat{u}_{\alpha})(B(\lambda, \hat{u}_{\beta}) + B(\lambda, \hat{u}_{\beta}')) + A(\lambda, \hat{u}_{\alpha}')(B(\lambda, \hat{u}_{\beta}') - B(\lambda, \hat{u}_{\beta})) = \pm \hbar^2/2 \quad (16.28)$$

We then define the quantity S as

$$S = E(\alpha, \beta) + E(\alpha, \beta') + E(\alpha', \beta') - E(\alpha', \beta)$$
(16.29)

and we get

$$\int P(\lambda)d\lambda \begin{bmatrix} A(\lambda, \hat{u}_{\alpha})B(\lambda, \hat{u}_{\beta}) + A(\lambda, \hat{u}_{\alpha})B(\lambda, \hat{u}_{\beta}') \\ +A(\lambda, \hat{u}_{\alpha}')B(\lambda, \hat{u}_{\beta}') - A(\lambda, \hat{u}_{\alpha}')B(\lambda, \hat{u}_{\beta}) \end{bmatrix}$$
$$= \frac{\hbar^{2}}{4} \left[E(\alpha, \beta) + E(\alpha, \beta') + E(\alpha', \beta') - E(\alpha', \beta) \right]$$
$$= \pm \frac{\hbar^{2}}{2} \int P(\lambda)d\lambda = \pm \frac{\hbar^{2}}{2}$$

or $|S| \leq 2$, which is Bell's inequality.

Now let us consider a special case $\alpha - \beta = \beta' - \alpha = \alpha' - \beta' = \pi/4$. The quantum mechanical result for S is

$$S_Q = -\cos(\alpha - \beta) - \cos(\alpha - \beta') - \cos(\alpha' - \beta') + \cos(\alpha' - \beta)$$
(16.30)

If we set $\theta_1 = \alpha - \beta$, $\theta_2 = \beta' - \alpha$, $\theta_3 = \alpha' - \beta'$, we can look for the extrema of

$$f(\theta_1, \theta_2, \theta_3) = \cos(\theta_1 + \theta_2 + \theta_3) - \cos\theta_1 - \cos\theta_2 - \cos\theta_3$$
(16.31)

The extrema correspond to $\theta_1 = \theta_2 = \theta_3$ and $\sin \theta_1 = \sin 3\theta_1$ whose solutions between 0 and π are $\theta_1 = 0$, $\pi/4$, $3\pi/4$, π .

Defining the function $g(\theta_1) = -3\cos\theta_1 + \cos 3\theta_1$ we have

$$g(0) = -2, g(\pi/4) = -2\sqrt{2}, g(3\pi/4) = 2\sqrt{2}, g(\pi) = 2$$
 (16.32)

The plot in Figure 16.2 below shows $g(\theta)$:



Figure 16.2: Bell Function

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The shaded areas correspond to results which *cannot* be explained by hidden variable theories. This system therefore constitutes a test of the predictions of quantum mechanics versus any local hidden variable theory.

16.3 The EPR(Einstein-Podolsky-Rosen) Argument-Quick Overview

The nondeterministic character of quantum mechanics is very disturbing for the classical physicist. Hence, there were repeated attempts to replace quantum theory by a statistical theory.

According to these theories, there exist hidden variables whose values prescribe the values of all observables for any particular object, except that the hidden variables are unknown to the experimenter, thus yielding the probabilistic character of the theory. The probabilistic character of quantum mechanics would then be quite analogous to that of classical statistical mechanics, where one can imagine that the motion of all the particles is, in principle, known.

For example, let us consider a particle of spin = 1/2 in an eigenstate of S_x with eigenvalue $\hbar/2$. According to quantum mechanics, the z-component is not fixed. If one measures it for a very large number of such particles, one finds $\hbar/2$ 50% of the time and $-\hbar/2$ 50% of the time. According to the idea of hidden variables, for each particle, parameters unknown to us would determine whether $\hbar/2$ or $-\hbar/2$ results. These hidden variables would prescribe $\pm \hbar/2$ each 50% of the time.

By means of a number of thought experiments, Einstein attempted to demonstrate the incompleteness of the quantum mechanical description and to get around the indeterminism and the uncertainty relation. Each of these arguments was refuted, in turn, by Bohr.

An argument - sometimes referred to as a paradox - due to Einstein, Podolsky and Rosen (EPR) , played a pivotal role in the discussion of indeterminism and the existence of hidden variables; we consider the argument as reformulated by David Bohm.

Let two spin = 1/2 particles in the singlet state

$$|0,0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right)$$
(16.33)

be emitted from a source an then move apart in space. Even if the two particles are separated by an arbitrarily large distance and can no longer communicate with one another, one finds the following correlations in this state during a measurement of the one particle spin states: If one measures the z-component of the spin and finds particle 1 spin up, particle 2 is spin down. If one finds particle 1 spin down, particle 2 has spin up.

If, instead, one measures S_x , then $+\hbar/2$ for particle 1 implies $-\hbar/2$ for particle 2, etc.

This expresses the *nonlocality* of quantum theory.

The experiment on particle 1 influences the result of the experiment on particle 2, although they are widely separated. The nonlocality is a consequence of the existence of correlated many-particle states such as the direct product

$$\uparrow\rangle\left|\downarrow\right\rangle \tag{16.34}$$

and the fact that one can linear superimpose such states.

The nonlocality of quantum mechanics does not lead to contradictions with relativity theory. Although a measurement of a spin component of particle 1 immediately reveals the value of that component for particle 2, no information can be transmitted in this way. Since particle 1 takes values $\pm \hbar/2$ each 50% of the time, this remains true for particle 2, even after the measurement of particle 1. Only by a subsequent(slow) comparison of the results is it possible to verify the correlation.

Einstein, Podolsky and Rosen gave the following argument in favor of hidden parameters in conjunction with the EPR thought experiment.

By the measurement of S_z or S_x of particle 1, the values of S_z or S_x of particle 2 are known. Because of the separation of the particles, there was no influence on particle 2, and therefore the values of S_z , S_x etc. must have been fixed before the experiment. Thus, there must be a more complete theory with hidden variables.

In the EPR argument, the predictions of the quantum states

$$|0,0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$$

are used, but the inherent nonlocality is denied.

In the remainder of our discussion, we will consider local hidden variables. These would predetermine which value each of the components of \vec{S} of particle 1 has and likewise for particle 2. Each of the particles would carry this information independently of the other.

16.3.1 The Bell Inequality again

We now show again that such local hidden variables lead to predictions different from those of quantum mechanics. We then compare the predictions with experiment.

We consider a correlation experiment in which a particle of total spin = 0 decays into two particles each with spin = 1/2. At a sufficiently large distance from the source, a rotatable polarizer and a detector are set up for each particle as shown below, so that the particles can be detected and we can investigate whether any correlation in the spin orientations exists. The setup is shown in Figure 16.3 below.

Figure 16.3: Bell-EPR Experiment

Polarizer 1 with angular setting α only lets particle 1 through if its spin in the direction \hat{n}_{α} has the value $+\hbar/2$ and polarizer 2 with angular setting β only lets particle 2 through if its spin in the direction \hat{n}_{β} has the value $+\hbar/2$. The particles are counted by detectors 1 and 2. If they respond, then the spin is positive, otherwise it is negative.

We consider the correlation between various angular settings of the polarization experiment.

A measure of the correlation is $N(\alpha; \beta)$, defined as the relative number of experiments resulting in particle 1 at angle α being positive and particle 2 at angle β being positive.

Using the spin projection operator

$$P_{\theta} = \frac{1}{2} \left(1 + \vec{\sigma} \cdot \hat{n}_{\theta} \right) \tag{16.35}$$

quantum mechanics gives

$$N(\alpha;\beta) = \langle 0,0 | \frac{1}{2} (1 + \vec{\sigma}_1 \cdot \hat{n}_\alpha) \frac{1}{2} (1 + \vec{\sigma}_2 \cdot \hat{n}_\beta) | 0,0 \rangle$$

= $\langle 0,0 | \frac{1}{2} (1 + \vec{\sigma}_1 \cdot \hat{n}_\alpha) \frac{1}{2} (1 - \vec{\sigma}_1 \cdot \hat{n}_\beta) | 0,0 \rangle$
= $\frac{1}{4} (1 - \hat{n}_\alpha \cdot \hat{n}_\beta)$ (16.36)

since $\langle 0, 0 | \vec{\sigma}_1 | 0, 0 \rangle = 0$ in the singlet state. For coplanar detectors this reduces to

$$N(\alpha;\beta) = \frac{1}{2}\sin^2\frac{\beta-\alpha}{2}$$
(16.37)

If hidden variables were really present, we could represent $N(\alpha;\beta)$ by the following sum

$$N(\alpha;\beta) = N(\alpha\gamma;\beta) + N(\alpha;\gamma\beta)$$
(16.38)

Here, $N(\alpha\gamma;\beta)$ is the relative number of particle pairs in which particle 1 has positive spin at angles α and γ and negative spin at β , while $N(\alpha;\gamma\beta)$ is the relative number of particle pairs in which particle 1 has negative spin at |gammainstead. In theories with hidden variables, all of these quantities are assumed to be known.

Now one has $N(\alpha\gamma;\beta) \leq N(\gamma;\beta)$ since $N(\gamma;\beta) = N(\alpha\gamma;\beta) + N(\gamma;\beta\alpha)$ and both quantities on the right-hand side of the equation are nonnegative. Similarly, $N(\alpha;\gamma\beta) \leq N(\alpha;\gamma)$. Thus,

$$N(\alpha;\beta) \le N(\alpha;\gamma) + N(\gamma;\beta) \tag{16.39}$$

This is a simple version of the *Bell inequality*.

Remarks

1. In experiments one often works with the correlation defined by

$$P(\alpha;\beta) = \langle 0,0 | \left(\vec{\sigma}_1 \cdot \hat{n}_\alpha\right) \left(\vec{\sigma}_2 \cdot \hat{n}_\beta\right) | 0,0 \rangle = 4N(\alpha;\beta) - 1$$
(16.40)

instead of $N(\alpha; \beta)$ itself. Using

$$N(\alpha;\beta) = \frac{1}{2}\sin^2\frac{\beta-\alpha}{2}$$
(16.41)

we get

$$P(\alpha - \beta) \equiv P(\alpha; \beta) = -\cos(\alpha - \beta)$$
(16.42)

and Bell's inequality becomes

$$P(\alpha;\beta) - 1 \le P(\alpha;\gamma) + P(\gamma;\beta) \tag{16.43}$$

2. The limit prescribed by the Bell inequality can be determined as follows. In

$$N(\alpha;\beta) \le N(\alpha;\gamma) + N(\gamma;\beta) \tag{16.44}$$

we substitute for α, β, γ the values $0, \pi, \pi/2$ respectively to obtain

$$N(0;\pi) \le N(0;\pi/2) + N(\pi/2;\pi) \tag{16.45}$$

In the singlet state,

$$N(0;\pi) = \frac{1}{2}$$
, $N(0;\pi/2) = N(\pi/2;\pi)$ (16.46)

so that

$$N(0;\pi/2) \ge \frac{1}{4} \tag{16.47}$$

Other values can be obtained by different combinations of angles.

Finally, we contrast the consequences of the Bell inequality with quantum mechanics and compare with experiments.

To this end, we compute $N(\alpha;\beta)$, $N(\alpha;\gamma)$ and $N(\gamma;\beta)$ for the three angles $\alpha = 0^{\circ}$, $\gamma = 45^{\circ}$ and $\beta = 90^{\circ}$ using

$$N(\alpha;\beta) = \frac{1}{2}\sin^2\frac{\beta-\alpha}{2}$$
(16.48)

to get

$$\frac{1}{2}\sin^2 45^\circ \le 2\sin^2 22.5^\circ \tag{16.49}$$

 \mathbf{or}

$$0.5 \le 0.29 \tag{16.50}$$

which is clearly not true! Therefore, quantum mechanics and hidden variables are incompatible.

The comparison of quantum mechanics and the Bell inequality is shown in Figure 16.4 below, which gives the correlation $P(\theta) = P(\theta; 0)$ according to quantum mechanics and the Bell inequality.



Figure 16.4: Bell-EPR Experiment Theoretical Predictions

The experimental demonstration of the violation of the Bell inequality by Lamehl-Rachti for protons and Aspect for photons is shown in Figure 16.5 below which gives the experimental results on the spin correlation of proton pairs



Figure 16.5: Bell-EPR Experiment - Data

Clearly, quantum mechanics is correct. This means that any theory that has the same probabilistic predictions as quantum mechanics must be *nonlocal*.

16.4 EPR and Bell - The Details

Let us first rethink some quantum mechanical ideas in a context needed for this discussion. This review will hopefully reinforce the ideas you have learned so far.

16.4.1 Single-Photon Interference

All good discussions on quantum mechanics present a long an interesting analysis of the double slit experiment. The crux of the discussion comes when the light intensity is reduced sufficiently for photons to be considered as presenting themselves at the entry slit one by one. For a long time this point was very contentious, because correlations between two successive photons cannot be ruled out a priori.

Since 1985, however, the situation has changed. An experiment was performed by Grangier, Roger and Aspect. It was an interference experiment with only a single photon. They used a light source devised for an EPR experiment which guarantees that photons arrive at the entry slit singly.

The experiment is difficult to do in practice, but is very simple in principle and

it provides an excellent experimental introduction to the concepts of quantum mechanics.

The light source is a beam of calcium atoms, excited by two focused laser beams having wavelengths $\lambda' = 406 nm$ and $\lambda'' = 581 nm$ respectively. Twophoton excitation produces a state having the quantum number J = 0. When it decays, this state emits two monochromatic photons having the wavelengths $\lambda_1 = 551.3 nm$ and $\lambda_2 = 422.7 nm$ respectively, in a cascade of two electronic transitions from the initial J = 0 level to the final J = 0 state, passing through an intermediate J = 1 state, as shown in Figure 16.6 below



Figure 16.6: Calcium based light source - Energy Levels

The mean lifetime of the intermediate state is 4.7 ns. To simplify the terminology, we shall call the $\lambda_1 = 551.3 nm$ light green, and the $\lambda_2 = 422.7 nm$ light violet.

Next we describe the experiment, exhibiting its three stages which reveal the complications of the apparatus in progressively greater detail (Figures 16.7-16.9 below).

1. The first stage is a trivial check that the apparatus is working properly; nevertheless it is already very instructive (Figure 16.7 below).

Figure 16.7 shows interference with a single photon (first stage). In the sketch, solid lines are optical paths and dashed lines are electrical connections.

On either side of the source S one positions two photomultiplier tubes PM_O and PM_A . These are very sensitive, and can detect the arrival of a single photon. Detection proceeds through photoelectric absorption, followed by amplification which produces an electric signal proportional



Figure 16.7: Single Photon Interference Experiment - Stage 1

to the energy of the incident photon. The associated electronic logic circuits can identify the photons absorbed by each detector: the channel PM_O responds only to green light, and the channel PM_A responds only to violet light. The electronic gate is opened (for 9 ns - this is twice the mean lifetime and corresponds to an 85% probability that the photon has been emitted) when green light is detected by PM_O . If, while the gate is open, violet light is emitted by the same atom towards(not all of the violet photons go towards the source) PM_A , then PM_A detects this photon, producing a signal that passes through the gate and is counted in N_A . The counter N_O registers the number of green photons detected by PM_O . It turns out that $N_A \ll N_O$. As the observation period becomes very long(approximately 5 hours), the ratio N_A/N_O tends to a limit that is characteristic of the apparatus. It represents the probability of detecting a violet photon in PM_A during the 9 ns following the detection of a green photon by PM_O .

The purpose of this arrangement is to use a green photon in order to open a 9ns time window, in which to detect a violet photon emitted by the same atom. As we shall see, there is only an extremely small probability of detecting through the same window another violet photon emitted by a different atom.

We will assume that a second observer is in the lab. This observer always feels compelled to present what he thinks are *simple-minded truths* using ordinary words. We will called this second observer Albert. Albert, as we shall see, has a tendency to use, one after another, the three phrases, *I observe*, *I conclude*, and *I envisage*. Consulted about the above experiment, Albert states, with much confidence,

I observe that the photomultiplier PM_A detects violet light when the source

S is on, and that it ceases to detect anything when the source is off. I conclude that the violet light is emitted by S, and that it travelled from S to PM_A .

I observe that energy is transferred between the light and the photomultiplier PM_A always in the same amount, which I will call a quantum.

I envisage the quanta as particles, emitted by the source, propagating freely from S to PM_A , and absorbed by the detector. I shall call this quanta photons.

Albert stops talking at this point.

2. The second stage of the experiment introduces the concept of individual photons in Figure 16.8 below which is interference with a single photon (second stage).



Figure 16.8: Single Photon Interference Experiment - Stage 2

Across the path of the violet light one places a half-silvered mirror LS_{α} , which splits the primary beam into two secondary beams(equal intensity), one transmitted and detected by PM_A , the other reflected and detected by PM_B . As in the first stage, the gate is opened for 9 ns, by PM_O . While it is open, one registers detection by either PM_A (counted as N_A) or by PM_B (counted as N_B) or by both, which we call a coincidence (counted as N_C). The experiment runs for 5 hours again and yields the following results:

- (a) The counts N_A and N_B are both of the order of 10⁵. By contrast, N_C is much smaller, being equal to 9.
- (b) The sequence of counts from PM_A is random in time, as is the sequence of counts from PM_B .

(c) The very low value of N_C shows that counts in PM_A and PM_B are mutually exclusive (do not occur at same time).

The experimenters analyze the value of N_C in depth; their reasoning can be outlined as follows:

- (a) Suppose two different atoms each emit a violet photon, one being transmitted to PM_A and the other reflected to PM_B with both arriving during the 9ns opening of the gate; then the circuitry records a coincidence. In the regime under study, and for a run of 5 hours, quantum theory predicts that the number of coincidences should be $N_C = 9$. The fact that this number is so small means that, in practice, any given single photon is either transmitted or reflected.
- (b) If light is considered as a wave, split into two by LS_{α} and condensed into quanta on reaching PM_A and PM_B , then one would expect the photon counts to be correlated in time, which would entail $N_C \gg 9$. Classically speaking this would mean that we cannot have a transmitted wave without a reflected wave.
- (c) Experiment yields $N_C = 9$; this quantum result differs from the classical value by 13 standard deviations; hence the discrepancy is very firmly established, and allows us to assert that we are indeed dealing with a source of individual photons.

Albert leaves such logical thinking to professionals. Once he notes that N_C is very small, he is quite prepared to treat it as if it were zero. He therefore says I observe that light travels from the source to PM_A or to PM_B , because detection ceases when the source is switched off.

I observe the counts N_A and N_B correspond to a game of heads or tails, in that the two possibilities are mutually exclusive, and that the counts are random.

I observe that the optical paths 1 and 2 are distinguishable, because the experiment allows me to ascertain, for each quantum, whether it has travelled path 1 (detection by PM_A) or path 2 (detection by PM_B).

I envisage that, on arrival at the half-silvered mirror, each photon from the source is directed at random either along path 1 or along path 2; and I assert that it is the nature of photons to play heads or tails..

Digression: The Mach-Zender Interferometer and Quantum Interference

(a) The next experiment uses a Mach-Zender interferometer so let us see how it operates.

Background information: Consider a single photon incident on

a 50-50 beam splitter (that is, a partially transmitting, partially reflecting mirror, with equal coefficients). Whereas classical electromagnetic energy divides equally, the photon is indivisible. That is, if a photon-counting detector is placed at each of the output ports (see Figure 16.9 below), only *one* of them clicks. Which one clicks is completely random (that is, we have no better guess for one over the other).



Figure 16.9: 50-50 Beam Splitter

The input-output transformation of the waves incident on 50-50 beam splitters and perfectly reflecting mirrors are shown in Figure 16.10 below.



Figure 16.10: Input/output Transformations

We can easily show that with these rules, there is a 50-50 chance of either of the detectors shown in the first figure above to click. According to the rules given in the figure

$$\psi_{1,out} = \frac{1}{\sqrt{2}}\psi_{in}$$
, $\psi_{2,out} = \frac{1}{\sqrt{2}}\psi_{in}$ (16.51)

since nothing enters port #2.

By our probability postulate the probability to find a photon at position 1 or 2 is

$$\begin{array}{l} P_{1,out} = \int \left| \psi_{1,out} \right|^2 dx = \frac{1}{2} \int \left| \psi_{in} \right|^2 dx = \frac{1}{2} \\ P_{2,out} = \int \left| \psi_{2,out} \right|^2 dx = \frac{1}{2} \int \left| \psi_{in} \right|^2 dx = \frac{1}{2} \end{array} \right\} \Rightarrow 50 - 50\% \ chance$$

Note: As we see from the experimental discussion below, the photon is found at one detector or the other, never both. The photon is indivisible. This contrasts with classical waves where half of the intensity goes one way and half the other; an antenna would also receive energy. We interpret this as the mean value of a large number of photons.

(b) Now we set up a Mach-Zender interferometer(shown in Figure 16.11 below):



Figure 16.11: Mach-Zehnder Interferometer

?The wave is split at beam-splitter b1, where it travels either path b1-m1-b2(call it the green path) or the path b1-m2-b2 (call it the blue path). Mirrors are then used to recombine the beams on a second beam splitter, b2. Detectors D1 and D2 are placed at the two output ports of b2.

Assuming the paths are perfectly balanced (that is equal length), we can show that the probability for detector D1 to click is 100% - no randomness!

To find the wavefunctions impinging on detectors D1 and D2 let us apply the transformation rules sequentially.

(1) Beamsplitter #1

$$\psi_{1,out} = \frac{1}{\sqrt{2}}\psi_{in} \quad , \quad \psi_{2,out} = \frac{1}{\sqrt{2}}\psi_{in}$$

(2) Propagation a distance L/2 along each path mean that the phase of the wavefunction changes by $e^{ikL/2}$ so that the wavefunctions are

$$\psi_{1,at-mirror} = \frac{1}{\sqrt{2}} e^{ikL/2} \psi_{in} \quad , \quad \psi_{2,at-mirror} = \frac{1}{\sqrt{2}} e^{ikL/2} \psi_{in}$$

(3) Reflection off mirrors means wavefunctions become

$$\psi_{1,after-mirror} = -\frac{1}{\sqrt{2}} e^{ikL/2} \psi_{in}$$

$$\psi_{2,after-mirror} = -\frac{1}{\sqrt{2}} e^{ikL/2} \psi_{in}$$
(16.52)

(4) Propagation a distance L/2 along each path mean that the phase of the wavefunction changes by $e^{ikL/2}$ so that the wavefunctions are

$$\psi_{1,at-b2} = \frac{1}{\sqrt{2}} e^{ikL} \psi_{in}$$
, $\psi_{2,at-b2} = \frac{1}{\sqrt{2}} e^{ikL} \psi_{in}$

(5) After beamsplitter #2

$$\begin{split} \psi_{out,1} &= \frac{\psi_{1,at-b2} + \psi_{2,at-b2}}{\sqrt{2}} = e^{ikL}\psi_{in} \\ \psi_{out,2} &= \frac{\psi_{1,at-b2} - \psi_{2,at-b2}}{\sqrt{2}} = 0 \end{split}$$

Therefore,

$$P_{1,out} = \int |\psi_{out,1}|^2 dx = \int |\psi_{in}|^2 dx = 1$$
$$P_{2,out} = \int |\psi_{out,2}|^2 dx = 0$$

Thus, we have a 100% chance of detector D1 firing and a 0% chance of detector D2 firing. There is no randomness.

(c) Classical logical reasoning would predict a probability for D1 to click given by

$$P_{D1} = P(transmission \ at \ b1|green \ path)P(green \ path)$$

+ $P(reflection \ at \ b2|blue \ path)P(blue \ path)$

Now we know that there is a 50-50 probability for the photon to take the blue or green path which implies that

$$P(green) = P(blue) = 1/2$$

Also with the particle incident at b2 along the green path there is a 50% chance of transmission and similarly for reflection of the blue path.

Therefore,

 $P(transmission \ at \ b2|green) = P(reflection \ at \ b2|blue) = 1/2$

and

$$P_{D1} = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2}$$

so that classical reasoning implies a 50-50 chance of D1 firing, that is, it is completely random!

The quantum case is different because the two paths which lead to detector D1 interfere. For the two paths leading to D1 we have

$$\psi_{total} = \frac{\frac{1}{\sqrt{2}} e^{ikL} \psi_{in} + \frac{1}{\sqrt{2}} e^{ikL} \psi_{in}}{\sqrt{2}}$$
$$P_{D1} = \int |\psi_{total}|^2 dx = P_{D1} = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = 1$$

where the last two terms are the so-called interference terms. Thus, $P_{D1} = 1$. The paths that lead to detector D2 destructively interfere so that $P_{D2} = 0$.

We now ask how would you set up the interferometer so that detector D2 clicked with 100% probability? How about making them click at random?

Leave the basic geometry the same, that is, do not change the direction of the beam splitters or the direction of the incident light.

We now want constructive interference for the paths leading to D2 and destructive interference for D1.

We can achieve this by changing the relative phase of the two paths by moving the mirror so that the path lengths are not the same.

Suppose we move the mirror on the green path (at an angle of 45°) so that the path lengths in the green path are both changed to $L + \Delta L$. We then have

$$\begin{split} \psi_{out,1} &= \frac{\frac{1}{\sqrt{2}} e^{ik(L+\Delta L)} + \frac{1}{\sqrt{2}} e^{ikL}}{\sqrt{2}} = \psi_{in} \\ \psi_{out,2} &= \frac{\frac{1}{\sqrt{2}} e^{ik(L+\Delta L)} - \frac{1}{\sqrt{2}} e^{ikL}}{\sqrt{2}} = \psi_{in} \end{split}$$

and

$$P_{D1} = \int dx |\psi_{2,out}|^2 = \frac{1}{4} \int dx |\psi_{in}|^2 |e^{ikL}|^2 |e^{ik\Delta L} + 1|^2$$

= $\frac{1}{4} (e^{ik\Delta L} + 1) (e^{ik\Delta L} + 1)^* = \frac{1}{4} (e^{ik\Delta L} + 1) (e^{-ik\Delta L} + 1)$
= $\frac{1}{4} (2 + e^{ik\Delta L} + e^{-ik\Delta L}) = \frac{1 + \cos(k\Delta L)}{2} = \cos^2\left(\frac{k\Delta L}{2}\right)$

Similarly we have

$$P_{D2} = \int dx |\psi_{1,out}|^2 = \frac{1}{4} \int dx |\psi_{in}|^2 |e^{ikL}|^2 |e^{ik\Delta L} - 1|^2$$

= $\frac{1}{4} (e^{ik\Delta L} - 1) (e^{ik\Delta L} - 1)^* = \frac{1}{4} (e^{ik\Delta L} - 1) (e^{-ik\Delta L} - 1)$
= $\frac{1}{4} (2 - e^{ik\Delta L} - e^{-ik\Delta L}) = \frac{1 - \cos(k\Delta L)}{2} = \sin^2\left(\frac{k\Delta L}{2}\right)$

Therefore, to achieve ${\cal P}_{D1}=0$ and ${\cal P}_{D2}=1$ we choose

$$k\Delta L = m\pi \quad (m \ odd) \Rightarrow \Delta L = m\frac{\pi}{k} = m\frac{\lambda}{2}$$

We can make the both random if

$$\cos^{2}\left(\frac{k\Delta L}{2}\right) = \sin^{2}\left(\frac{k\Delta L}{2}\right) = \frac{1}{2} \Rightarrow \frac{k\Delta L}{2} = p\frac{\pi}{4} \quad (p \text{ odd})$$
$$\Delta L = p\frac{\pi}{2k} = p\frac{\lambda}{4}$$

Returning to our discussion.....

3. The third stage then consists of an interference experiment as shown in Figure 16.12 below, which is the interference with a single photon (third stage).



Figure 16.12: Mach-Zehnder Interferometer Inserted

A so-called Mach-Zehnder interferometer is used, allowing one to obtain two interference profiles. The beam of violet light from the source Sis split into two by the mirror LS_{α} . After reflection from two different mirrors, these secondary beams meet on a second half-silvered mirror LS_{β} . Here, each secondary beam is further split into two; thus one establishes two interference regions, region (1',2') where one places PM_A , and region (1",2") where one places PM_B .

A very high precision piezoelectric system allows one of the mirrors to be displaced so as to vary the path difference between the two arms of the interferometer. In this way one can shift the pattern of interference fringes by regular steps, without moving the detectors PM_A and PM_B ; the standard step corresponds to a change of $\lambda/50$ in the difference between the two optical paths.

A sweep, taking 15 sec for each standard step, yields two interference plots corresponding, respectively, to the paths (1',2') and (1'',2''); the fringes have good contrast(difference in intensity between maxima and minima), and their visibility

$$(N_{A,\max} - N_{A,\min}) / (N_{A,\max} + N_{A,\min})$$
 (16.53)

was measured as 98% as shown in Figure 16.13 below which gives the two interference plots obtained with the Mach-Zehnder interferometer. Note that the maximum counting rates in PM_A correspond to minima in PM_B , indicating a relative displacement of $\lambda/2$ between the two interference patterns



Figure 16.13: Interference Results

If we recall that we are reasoning in terms of photons, and that the photons are being processed individually, then we must admit that the interference does not stem from any interaction between successive photons, but that each photon interferes with itself.

What would Albert have to say? He seems exasperated but is still polite. His statements are brief:

I observe that the optical paths differ in length between LS_{α} and LS_{β} , and are then coincident over (1',2') and over (1'',2'').

In PM_A I observe a process that seems perfectly natural to me, namely

$$light + light \rightarrow light$$

In PM_B I observe a process that I find astounding, namely

 $light + light \rightarrow darkness$

Such superposition phenomena with light I shall call interference; constructive in PM_A and destructive in PM_B .

In the situation considered before, I envisaged light as consisting of particles called photons, which travelled either along path 1 or along path 2. In the present situation I want to know for each individual photon which path it has travelled; to this end I should like to ask you to close off path 2, since this will ensure that the photons travel by path 1..

Clearly Albert is perturbed. He awaits the new experimental results with some anxiety.

On closing either path, whether 1 or 2, one observes that all interference phenomena disappear. For instance, instead of a very high count N_A and a very low count N_B , we now obtain essentially equal counts from PM_A and PM_B .

Albert is visibly displeased and now very wary. He then continues with his analysis of the experiment:

I observe that in order to produce interference phenomena it is necessary to have two optical paths of different lengths, both open.

Whenever a photon is detected, I note my inability to ascertain whether the light has travelled by path 1 or by path 2, because I have no means for distinguishing between the two cases.

If I were to suppose that photons travel only along 1, then this would imply that path 2 is irrelevant, which is contrary to what I have observed. Similarly, if I were to suppose that photons travel only along 2, then this would imply that path 1 is irrelevant, which is also contrary to my observations.

If I envisage the source S as emitting particles, then I am forced to conclude that each individual photon travels simultaneously along both paths 1 and 2; but this result contradicts the results of the previous experiment (second stage), which compelled me to envisage that every photon chooses, at random, either path 1 or path 2.

I conclude that the notion of particles is unsuited to explaining interference phenomena.

I shall suppose instead that the source emits a wave; this wave splits into two at LS_{α} , and the two secondary waves travel one along path 1 and the other along path 2. They produce interference by mutual superposition on LS_{β} constructively in (1',2') and destructively in (1",2"). At the far end of (1',2') or of (1",2") I envisage each of the waves condensing into particles, which are then detected by the photomultipliers (essentially by PM_A since the contrast is 98% means only very few photons are detected by PM_B

It seems to me that I am beginning to understand the situation. I en-

visage light as having two complementary forms: depending on the kind of experiment that is being done, it can manifest itself either as a wave, or as a particle, but never as both simultaneously and in the same place. Thus, in the experiment where the path followed by the light cannot be ascertained (third stage), light behaves first like a wave, producing interference phenomena; but it behaves like a particle when, afterwards, it is detected through the photoelectric effect. I conclude that light behaves rather strangely, but nevertheless I have the impression that its behavior can be fully described once one has come to terms with the idea of wave-particle duality..

Albert leaves the room slowly, hesitantly, even reluctantly. He might be impressed by all the completeness of all that he has just described or maybe he is worried that more needs to be said.

In fact, something does remain to be said, since the problem of causality remains open. Let us look carefully at the experimental layouts in the second and third stages: we see that they have LS_{α} in common, and that they differ only beyond some boundary (indicated by the dashed circle downstream from LS_{α}). We have stated that light behaves like a particle or like a wave depending on whether or not one can ascertain the path it takes through the apparatus; but in the two experiments under consideration, the choice between the alternatives must be decided on LS_{α} , before the light has crossed the crucial boundary, that is, at a stage where nothing can as yet distinguish between the two kinds of apparatus, since they differ only beyond the point of decision. It is as if the light chose whether to behave like a wave or like a particle before knowing whether the apparatus it will pass through will elicit interference phenomena or the photoelectric effect. Hence the question of causality is indeed opened up with vengeance.

Albert comes back abruptly. He is disconcerted and wearily says:

Originally I supposed that light would behave like a wave or like a particle, depending on the kind of experiment to which it was being subjected.

I observe that the choice must be made on the half-silvered mirror LS_{α} , before the light reaches that part of the apparatus where the choice is actually implemented; this would imply that the effect precedes the cause.

I know that both waves and particles obey the principle of causality, that is, that cause precedes effect.

I conclude that light is neither wave nor particle; it behaves neither like waves on the sea, nor like projectiles fired from a gun, nor like any other kind of object that I am familiar with. I must ask you to forget everything I have said about this experiment, which seems to me to be thoroughly mysterious.

Albert leaves, but quickly returns with a contented smile, and his final statement is not without a touch of malice. I observe in all cases that the photomultipliers register quanta when I switch on the light source.

I conclude that "something" has travelled from the source to the detector. This "something" is a quantum object, and I shall continue to call it a photon, even though I know that it is neither a wave nor a particle.

I observe that the photon gives rise to interference when one cannot ascertain which path it follows; and that interference disappears when it is possible to ascertain the path.

For each detector, I observe that the quanta it detects are randomly distributed in time.

If I repeat the experiment several times under identical conditions, then I observe that the photon counts registered by each photomultiplier are reproducible in a statistical sense. For example, suppose that in the first and in the second experiments PM_A registers N'_A and N''_A respectively; then one can predict that N''_A has a probability of 0.68 of being in the interval $N'_A \pm (N'_A)^{1/2}$

Thus, these counts enable me to determine experimentally, for any kind of apparatus, the probability that a given detector will detect a quantum, and it is precisely such probabilities that constitute the results of experiments.

I assert that the function of a physical theory is to predict the results of experiments.

What I expect from theoretical physicists is a theory that will enable me to predict, through calculation, the probability that a given detector will detect a photon. This theory will have to take into account the random behavior of the photon, and the absence or presence of interference phenomena depending on whether the paths followed by the light can or cannot be ascertained..

Albert leaves, wishing the physicists well in their future endeavors.

Physicist have indeed worked hard and the much desired theory has indeed come to light, namely, quantum mechanics, as we have seen in our discussions. As we have seen, it applies perfectly not only to photons, but equally well to electrons, protons, neutrons, etc; in fact, it applies to all the particles of microscopic physics. For the last 75 years it has worked to the general satisfaction of physicists.

Meanwhile, it has produced two very interesting problems of a philosophical nature.

- 1. Chance as encountered in quantum mechanics lies in the very nature of the coupling between the quantum object and the experimental apparatus. No longer is it chance as a matter of ignorance or incompetence: it is *chance quintessential and unavoidable*.
- 2. Quantum objects behave quite differently from the familiar objects of our everyday experience: whenever, for pedagogical reasons, one allows an analogy with macroscopic models like waves or particles, one always fails sooner or later, because the analogy is never more than partially valid. Accordingly, the first duty of a physicist is to force her grey cells, that is her concepts and her language, into unreserved compliance with quantum mechanics (as we have been attempting to do); eventually this will lead her to view the actual behavior of microsystems as perfectly normal. As a teacher of physics, our duties are if anything more onerous still, because we must convince the younger generations that quantum mechanics is not a branch of mathematics, but an expression of our best present understanding of physics on the smallest scale; and that, like all physical theories, it is predictive.

In this context, let us review the basic formalism of quantum mechanics.

16.4.2 Basic Formalism

We will introduce the elements of quantum mechanics as axioms. Physicists have devised a new mathematical tool. The transition amplitude from initial to final state, and it is this amplitude that enables one to calculate the needed probabilities.

1. For the experiment where the photon travels from the source S to the detector PM_A (see Figure 16.14(a) below), we write the transition amplitude from S to PM_A as

 $\langle \text{photon arriving at } PM_A \mid \text{photon leaving S} \rangle$

which we symbolize simply as

$$\langle f_1 \mid i \rangle$$
 , $\langle f_2 \mid i \rangle$

In this case there are two probabilities:

$$\langle f_1 | i \rangle |^2$$
 , $|\langle f_2 | i \rangle |^2$

The total probability is their sum:

$$\left|\left\langle f_{1} \mid i\right\rangle\right|^{2} + \left|\left\langle f_{2} \mid i\right\rangle\right|$$

More generally, we would write

$$\left|\left\langle f \mid i\right\rangle\right|^2 = \sum_k \left|\left\langle f_k \mid i\right\rangle\right|^2$$

Figure 16.14 below shows three arrangements sufficient to determine the transition amplitude: (a) a single optical path; (b) two paths, allowing us to ascertain which path has actually been taken; (c) two paths, not allowing us to ascertain which path has actually been taken.



Figure 16.14: Three Arrangements

2. If a photon is emitted by the source S can take either of two paths, but it is impossible to ascertain which path it does take (Figure 16.14(c) above), then there are again two transition amplitudes:

 $\langle \text{photon arriving at } PM_A \mid \text{photon leaving S} \rangle_{\text{along path 1}}$

 $\langle photonarrivingat PM_B | photon leaving S \rangle_{along path 2}$

which we symbolize simply as

$$\left\langle f \mid i \right\rangle_1 \quad , \quad \left\langle f \mid i \right\rangle_2$$

To allow for interference, we assert that in this case it is the amplitudes that must be added; the total amplitude reads

$$\langle f \mid i \rangle = \langle f \mid i \rangle_1 + \langle f \mid i \rangle_2$$

The total probability is then:

$$\left|\left\langle f \mid i\right\rangle_1 + \left\langle f \mid i\right\rangle_2\right|^2$$

More generally, we would write

total amplitude:
$$\langle f \mid i \rangle = \sum_{k} \langle f \mid i \rangle_{k}$$

total probability: $|\langle f \mid i \rangle|^{2} = \left| \sum_{k} \langle f \mid i \rangle_{k} \right|^{2}$

where the sums are over all possible paths.

3. If one wants to analyze the propagation of the light more closely, one can take into account its passage through the half-silvered mirror LS_{α} , considering this as an intermediate state (Figure 16.14(b) above). The total amplitude for path 1 is

 $\langle \text{photon arriving at } PM_A \mid \text{photon leaving S} \rangle$

However, it results from two successive intermediate amplitudes:

 $\langle \text{photon arriving at } LS_{\alpha} \mid \text{photon leaving } S \rangle$ $\langle \text{photon arriving at } PM_A \mid \text{photon leaving } LS_{\alpha} \rangle$

Here we consider the total amplitude as the product of the successive intermediate amplitudes; symbolically, labelling the intermediate state as v, we have

 $\langle f \mid i \rangle = \langle f \mid \nu \rangle \langle \nu \mid i \rangle$

Finally, consider a system of two mutually independent photons. If photon 1 undergoes a transition from a state i_1 to a state f_1 , and photon 2 from a state i_2 to a state f_2 , then

$$\langle f_1 f_2 \mid i_1 i_2 \rangle = \langle f_1 \mid i_1 \rangle \langle f_2 \mid i_2 \rangle$$

The four rules just given suffice to calculate the detection probability in any possible experimental situation. They assume their present form as a result of a long theoretical evolution; but they are best justified *a posteriori*, because in 75 years they have never been found to be wrong. Accordingly, we may consider them as the basic principles governing the observable behavior of all microscopic objects, that is, objects whose action on each other are of order (Planck's constant). From these principles (they are equivalent to our earlier postulates - just look different because we are using the amplitude instead of the state vector as the fundamental mathematical object in the theory) one can derive all the requisite formalism, that is, all of quantum mechanics.

Quantum mechanics as we have described it earlier and also above, works splendidly, like a well-oiled machine. It, and its basic principles, might therefore be expected to command the assent of every physicist; yet it has evoked, and on occasion continues to evoke, reservations both explicit and implicit. For this there are two reasons:

- 1. Quantum mechanics introduces unavoidable chance, meaning that its characteristic randomness is inherent in the microscopic phenomena themselves.
- 2. It attributes to microscopic objects properties so unprecedented that we cannot represent them through any macroscopic analogs or models.

Both features are revolutionary, and it is natural that they should have provoked debate. On the opposite sides of this debate we find two great physicists, Neils Bohr and Albert Einstein, and we will now discuss how the debate evolved from its beginnings in 1927 to its conclusion in 1983 (that is 56 years!).

16.5 Inseparable Photons (the EPR Paradox) including some history

Though ornithologists have known about inseparable parrots for a long time, to physicists the existence of inseparable photons has been brought home only during the last two decades, through a beautiful series of experiments by Alain Aspect and his research group at Orsay Laboratory in Paris. The experiments are exemplary, in virtue both of the difficulties they had to overcome and the results achieved, which are exceptionally clear-cut. In fact, the significance of the experiments extends beyond the strict confines of physics, because they provide the touchstone for settling a philosophical debate that has divided physicist for 75 years. The division dates back to the appearance of two mutually contradictory interpretations of quantum mechanics at the Como conference in 1927. To sketch the debate, we start with a brief summary of the philosophy of physics.

16.5.1 The Philosophical Stakes in the Debate

Our summary is best presented diagrammatically as shown in Figure 16.15 below where we present the philosophical elements in a debate between physicists.



Figure 16.15: Philosophical Ideas

- 1. For the physicist who is a *realist*, a physical theory reflects the behavior of real objects, whose existence is not brought into question.
- 2. For the physicist who is a *positivist*, the purpose of a physical theory is to describe the relations between measurable quantities. The theory does not tell one whether anything characterized by these quantities really exists, nor even whether the question makes sense.
- 3. For the physicist who is a *determinist*, exact knowledge of the initial conditions and of the interactions allows the future to be predicted exactly. Determinism is held to be a universal characteristic of natural phenomena, even about those which we know, as yet, little or nothing. In this framework, any recourse to chance merely reflects our own ignorance.
- 4. For the physicist who is a *probabilist*, chance is inherent in the very nature of microscopic phenomena. To her, determinism is a consequence, on the macroscopic level, if the laws of chance operating on the microscopic level; it is appropriate to measurements of mean values of quantities whose relative fluctuations are very weak.

From these four poles, realism, positivism, determinism, and chance, the physicist chooses two, one on each axis. Though sometimes the choice is made in full awareness of what it entails, most often it is made subconsciously. In our description of quantum mechanics, we might adopt without reservations, the point of view of the elementary particle physicist. For a start, she believes firmly in the existence of particles, since she spends her time in accelerating, deflecting, focusing, and detecting them. Even though she has never seen or touched them, to her their objective existence is not in any doubt. Next she observes that they impinge on the detectors quite erratically, whence she has no doubts, either, that their behavior is random. Accordingly, the elementary particle experimentalist has chosen realism and chance, most often without realizing that she has made choices at all.

There are other philosophical options that can be adopted with eyes fully open: realism and determinism are the choices of Albert Einstein; positivism and chance are those of Neils Bohr. They are well acquainted and each thinks very highly of the other: which is no bar to their views being incompatible, nor to the two men representing opposite poles of the debate.

16.5.2 From Como to Brussels (1927-30)

On September 26,1927, in Como, Niels Bohr delivered a memorable lecture. His stance is that of an enthusiastic champion of the new quantum mechanics. He puts special weight on the inequalities proved by Heisenberg the year before:

$$\Delta x \Delta p_x \ge \frac{1}{2}\hbar$$
 , $\Delta t \Delta E \ge \frac{1}{2}\hbar$ (16.54)

They imply that it is impossible to define exact initial conditions for a microscopic object, which automatically makes it impossible to construct, on the microscopic scale, a deterministic theory patterned on classical mechanics. Only a probabilistic theory is possible, and that theory is quantum mechanics.

Einstein disagrees with this point of view, and his opposition to Bohr's theses becomes public at the Brussels conference in 1930: he adopts the role of a dissenter who knows precisely how to press home the most difficult questions. Deeply shocked by the retreat from determinism, he tries to show via his thought (gedanken) experiments he can contravene the Heisenberg inequalities.

At the cost of several sleepless nights devoted to analyzing the objections of his adversary, Bohr refutes all of Einstein's criticisms, and emerges from the conference as the undoubted winner.

16.5.3 From Brussels to the EPR Paradox (1930-35)

Having lost the argument at Brussels, Einstein tries to define his objections with ever greater precision. Believing as he does that position and momentum exist emphobjectively and simultaneously, he considers quantum mechanics to be incomplete and merely provisional. The points of view of the two antagonists at this stage of the debate can be spelled out as follows.

For Einstein, a physical theory must be a deterministic and a complete representation of the objective reality underlying the phenomena. It features known variables that are observable, and others, unknown as yet, called *hidden variables*. Because of our provisional ignorance of the hidden variables, matter at the microscopic level appears to us to behave arbitrarily, and we describe it by means of a theory that is incomplete and probabilistic, namely by quantum mechanics.

For Bohr, a physical theory makes sense only as a set of relations between observable quantities. Quantum mechanics supplies a correct and complete description of the behavior of objects at the microscopic level, which means that the theory itself is likewise complete. The observed behavior is probabilistic, implying that chance is inherent in the nature of the phenomena.

Between chance as a matter of ignorance, as advocated by Einstein, and chance unavoidable, as advocated by Bohr, the debate does not remain merely philosophical. Quite naturally it returns to the plane of physics with the thought experiment proposed by Einstein, Podolsky and Rosen in 1935, which in their view proves that quantum mechanics is indeed incomplete. Their thought experiment is published as a paper in the Physical Review, but it is so important that it reverberates as far as the New York Times. Physicists call the proposal the EPR paradox, after its proponents. It will take fifty years to untangle the question, first in theory and then by experiment. We will not, of course, follow these fifty years blow by blow; instead, we confine attention to three decisive stages reached respectively in 1952, 1964, and 1983. But we start with an illustration that helps one see what the EPR paradox actually is.

16.5.4 Elementary Introduction to the EPR Paradox

Consider two playing cards, one red(diamond) and one black(spade) as shown in Figure 16.16 below where we use two playing cards help us understand the stakes in the EPR paradox.



Figure 16.16: EPR Setup

An experimenter in Lyons puts them into separate envelopes which she then seals. She is thus provided with two envelopes looking exactly alike, and she puts both into a container. She shakes the container so as the *shuffle the pack*, and the system is ready for the experiment.

At 8:00 two travellers, one from Paris and one from Nice, come to the container (in Lyons), take one envelope each, and then return to Paris and Nice, respectively. At 14:00 they are back at their starting points; each opens her envelope, looks at the card, and telephones to Lyons reporting the color. The experiment is repeated every day for a year, and the observer in Lyons keeps a careful record of the results. At the end of the year the record stands as follows:

- 1. The reports from Paris are *red* or *black*, and the sequence of these reports is random. The situation is exactly the same as in a game of heads or tails, and probability of each outcome is 1/2.
- 2. The reports from Nice are *red* or *black*, and the sequence of these reports is random. Here too probability of each outcome is 1/2.
- 3. When Paris reports *red*, Nice reports *black*; when Paris reports *black*, Nice reports *red*. One sees that there is perfect(anti) correlation between the report from Paris and the report from Nice.

Accordingly, the experiment we have described displays two features:

- 1. It is *unpredictable* and thereby random at the level of individual observations in Paris and Nice.
- 2. It is *predictable*, by virtue of the correlation, at the level where one observes the Paris and the Nice results simultaneously.

Einstein and Bohr might have interpreted the correlation as follows.

According to Einstein

The future of the system is decided at 8:00 when the envelopes are chosen, because he believes that the contents of the two envelopes differ. Suppose, for instance, that Paris has (without knowing it) drawn a red card, and Nice the black. The colors so chosen exist in reality, even though we do not know them. The two cards are moved, separately, by the travellers between 8:00 and 14:00, during which time they do not influence each other in any way. The results on opening the envelopes read *red* in Paris and *black* in Nice. Since the choice at 8:00 was made blind, the opposite outcome is equally possible, but the results at 14:00 are always correlated (either red/black or black/red). This correlation at 14:00 is determined by the separation of the colors at 8:00, and we say the theory proposed by Einstein is *realist, deterministic, and separable(or local)*, by virtue of a hidden variable, namely, the color.

According to Bohr

There is a crucial preliminary factor, inherent in the preparation of the system. On shaking the container with the two envelopes, one loses information regarding the colors. Afterwards, one only knows that each envelope contains either a red card (probability 1/2) or a black card (probability 1/2). We will therefore say that a given envelope is in a *brown state*, which is a superposition of a red state and of a black state having equal probabilities. At 8:00 the two envelopes are identical: both are in a *brown state*, and the future of the system is still undecided. There is no solution until the envelopes are opened at 14:00, since it is only the action of opening them that makes the colors observable. The result is probabilistic. There is a probability 1/2 that in Paris the envelope will be observed to go from the *brown state* to the red, while the envelope in Nice is observed to go from the *brown state* to the black; there is the same probability 1/2 of observing the opposite. But the results of the observations on the two envelopes are always correlated, which means that there is a mutual influence between them, in particular at 14:00; in fact it is better to say that, jointly, they constitute a single and non-separable system, even though one is in Paris and the other is in Nice. Accordingly, the theory proposed by Bohr is positivist, probabilistic (non-deterministic) and non-separable (non-local), interrelating as it does the colors that are actually observed.

Einstein's view appears to be common sense, while it must be admitted that Bohr's is very startling; however, the point of this macroscopic example is, precisely, to stress how different the quantum view is from the classical.

Proceeding with impeccable logic but from different premises, both theories predict the same experimental results. Can we decide between them? At the level considered here it seems we cannot: for even if the envelopes were opened prematurely while still in Lyons, one would merely obtain the same results at a different time, and without affecting the validity of either interpretation. The solution to the problem must be looked for at the atomic level, by studying the true EPR set-up itself.

16.5.5 The EPR Paradox (1935-52)

Albert Einstein, Boris Podolsky, and Nathan Rosen meant to look for an experiment that could measure, indirectly but simultaneously, two mutually exclusive quantities like position and momentum. Such results would contravene the predictions of quantum mechanics, which allows the measurement of only one such quantity at any one time; that is why the thought experiment is called the EPR paradox.

In 1952, David Bohm showed that the paradox could be set up not only with continuously varying quantities like position and momentum, but also with discrete quantities like spin. This was the first step towards any realistically conceivable experiment. Meanwhile, objectives have evolved, and nowadays it is more usual to talk of the EPR scenario, meaning some sensible experiment capable of discriminating between quantum theory and hidden-variable theories. Such a set-up is sketched in Figure 16.17 below where we present the simplest EPR scenario.



Figure 16.17: EPR Scenario

A particle with spin 0 decays, at S, into two particles of spin 1/2, which diverge from S in opposite directions. Two Stern-Gerlach type detectors A and B measure the x-components of the spins. Two types of response are possible:

1. spin up at A, spin down at B, a result denoted by (+1, -1)

2. spin down at A, spin up at B, a result denoted by (-1, +1)

Thus far everyone is agreed, but the interpretation is yet to come.

Einstein reasons that if pairs of particles produced at S elicit different responses (+1, -1) and (-1, +1) from the detector system A,B, then the pairs must have differed already at S, immediately after the decay.

It must be possible to represent this difference by a hidden variable λ , which has an objective meaning, and *which governs the future of the system*. After the decay the two particles separate without influencing each other any further, and eventually they trigger the detectors A and B.

Bohr reasons that all the pairs produced at S are identical. Each pair constitutes a non-separable system right up to the time when the photons reach the detectors A and B. At that time we observe the response of the detectors, which is probabilistic, admitting two outcomes (+1, -1) and (-1, +1). To sum up, Einstein restricts the operation of chance to the instant of decay (at S), whose details we ignore, but which we believe creates pairs whose hidden variables λ are different.

By contrast, Bohr believes that chance operates at the instant of detection, and that it is inherent in the very nature of the detection process: this chance is unavoidable.

We are still in the realms of thought, and stay there up to 1964.

In 1964, the landscape changes: John Bell, a theorist at CERN, shows that it is possible to distinguish between the two interpretations experimentally.

The test applies to the EPR scenario; it is refined by Clauser, Horne, Shimony, and Holt, whence it is called the BCHSH inequality after its five originators.

16.5.6 The BCHSH Inequality (1964)

To set up an EPR scenario, one first needs a source that emits particle pairs. Various experimental possibilities have been explored:

- 1. atoms emitting two photons in cascade
- 2. electron-positron annihilation emitting two high-energy photons
- 3. elastic proton-proton scattering

It is solution (1) that has eventually proved the most convenient; it has been exploited by Alain Aspect at the Institute for Optics in Paris, in particular.

Next one needs detectors whose response can assume one of two values, represented conventionally by +1 and -1. Such a detector might be

- 1. for spin 1/2 particles, a Stern-Gerlach apparatus responding to spin up or spin down
- 2. for photons, a polarizer responding to *parallel polarization* or *perpendicular* polarization

Our sketch of the EPR scenario can now be completed as in Figure 16.18 below where we present the most general EPR scenario.



Figure 16.18: BCHSH Setup

Figure 16.18(a) views the apparatus perpendicularly to axis, showing the two detectors A and B, with their polarizing directions denoted as \vec{A} and \vec{B} .

Figure 16.18(b) views the apparatus along its axis, and shows that the analyzing directions of the two detectors are not parallel, but inclined to each other at an angle θ .

In Figure 16.18((c) we also a view along the axis of the apparatus, and shows the actual settings chosen by Aspect: two orientations are allowed for each detector, \vec{A}_1 or \vec{A}_2 for one, and \vec{B}_1 or \vec{B}_2 for the other.

We adopt the following conventions:

- (1) $\alpha = \pm 1$ is the response of detector A when oriented along \vec{A}
- (2) $\beta = \pm 1$ is the response of detector B when oriented along \vec{B}

Since each detector has two possible orientations, called 1 and 2, we shall denote their responses as α_1, α_2 and β_1, β_2 respectively. Now consider the quantity $\langle \gamma \rangle$ defined by

$$\langle \gamma \rangle = \langle \alpha_1 \beta_1 \rangle + \langle \alpha_1 \beta_2 \rangle + \langle \alpha_2 \beta_1 \rangle - \langle \alpha_2 \beta_2 \rangle \tag{16.55}$$

where the symbol $\langle ... \rangle$ denotes the mean value over very many measured events. We call $\langle \gamma \rangle$ the *correlation function* of the system.

The BCHSH inequality reads $-2 \leq \langle \gamma \rangle \leq 2$. Its authors have proved that it must be satisfied if mechanics at the microscopic level constitutes a theory that is realist, deterministic, and separable: or in other words if the theory contains a hidden variable. A sketch of the a proof is shown below.

A Proof of Bell's Inequality

A theory that is deterministic and separable

Suppose that the pair a, b emerging from S can be characterized by a hidden variable λ . The responses of the detectors A, B are $\alpha(\vec{A}, \lambda)$ and $\beta(\vec{B}, \lambda)$ respectively as shown in Figure 16.19 below.



Figure 16.19: Bell Inequality Setup

The theory is deterministic and separable:

- 1. deterministic, because the results are determined by the hidden variables plus the settings \vec{A} and \vec{B}
- 2. *separable*, because the response of A is independent of the response of B, and vice versa

Since the value of λ is unknown and different for each pair, the responses of A and B seem random. Lacking information about λ , we characterize it by choosing a statistical distribution $\rho(\lambda)$, which then allows us to derive the distribution of the responses $\alpha(\vec{A}, \lambda)$ and $\beta(\vec{B}, \lambda)$, which can be compared with experiment.

Bell's inequalities have the great virtue that they apply to any hidden variable theory, irrespective of the choice of $\rho(\lambda)$.

Theorem 1: Consider the four numbers α_1, α_2 and β_1, β_2 , each of which can assume only the values 1 or -1. Then the combination

$$\gamma = \alpha_1 \beta_1 + \alpha_1 \beta_2 + \alpha_2 \beta_1 - \alpha_2 \beta_2 \tag{16.56}$$

can assume only the values 2 and -2.

To prove the theorem, one constructs a truth table for all 16 possibilities, which

| α_1 | α_2 | β_1 | β_1 | γ |
|------------|------------|-----------|-----------|----------|
| 1 | 1 | 1 | 1 | 2 |
| 1 | 1 | 1 | -1 | 2 |
| 1 | 1 | -1 | 1 | -2 |
| 1 | 1 | -1 | -1 | -2 |
| 1 | -1 | 1 | 1 | 2 |
| 1 | -1 | 1 | -1 | 2 |
| 1 | -1 | -1 | 1 | -2 |
| 1 | -1 | -1 | -1 | -2 |
| -1 | 1 | 1 | 1 | -2 |
| -1 | 1 | 1 | -1 | 2 |
| -1 | 1 | -1 | 1 | -2 |
| -1 | 1 | -1 | -1 | 2 |
| -1 | -1 | 1 | 1 | -2 |
| -1 | -1 | 1 | -1 | -2 |
| -1 | -1 | -1 | 1 | 2 |
| -1 | -1 | -1 | -1 | 2 |

Table 16.1: γ Values

shows that 2 and -2 are indeed the only possible values of γ . **Theorem 2**: Consider very many sets of four numbers α_1, α_2 and β_1, β_2 . The mean value of γ lies in the range [-2, 2]. In other words,

$$-2 \le \langle \gamma \rangle \le 2 \tag{16.57}$$

This is obvious, because every value of γ lies in this range, and so therefore must the mean. The endpoints are included in order to allow for limiting cases. Note that both theorems are purely mathematical, neither involves any assumptions about physics.

16.5.7 BCHSH Inequality(Bell's inequality in real world)

Within the framework of a theory that is realist, deterministic, and separable, we can describe the photon pair in detail. Realism leads us to believe that polarization is an objective property of each member of the pair, independent of any measurements that may be made later. Determinism leads us to believe that the polarizations are uniquely determined by the decay cascade, and that they are fully specified by the hidden variable λ , which governs the correlation of the polarizations in A and B. Finally, separability leads us to believe that the measurements in A and B do not influence each other, which means in particular that the response of detector A is independent of the orientation of detector B.

Now consider a pair of photons a, b, characterized by a hidden variable λ . The

response of the apparatus in its four settings would be as follows:

 α_1 and β_1 in the orientation (\vec{A}_1, \vec{B}_1) α_2 and β_2 in the orientation (\vec{A}_2, \vec{B}_2) α'_1 and β'_2 in the orientation (\vec{A}_1, \vec{B}_2) α'_2 and β'_1 in the orientation (\vec{A}_2, \vec{B}_1)

Recall that the variables α and β can only take on the values 1 and -1. It is impossible in practice to make four measurements on one and the same pair of photons, because each photon is absorbed in the first measurement made on it; that is why we have spoken conditionally, that is, of what results would be(a **COUNTERFACTUAL** statement). But if we believe that the photon correlations are governed by a theory that is realist, deterministic, and separable, then we are entitled to assume that the responses, of type α or type β , depend on properties that the photons possess before the measurement, so that the responses correspond to some objective reality. In such a framework we can appeal to the principle of separability, which implies, for instance, that detector A would give the same response to the orientations (\vec{A}_1, \vec{B}_1) and (\vec{A}_1, \vec{B}_2) , because the response of A is independent of the orientation of B.

Mathematically, this is expressed by the relation $\alpha_1 = \alpha'_1$.

Similarly one finds $\alpha_2 = \alpha'_2$, $\beta_1 = \beta'_1$, $\beta_2 = \beta'_2$.

Thus, we have shown that, for a given pair of photons, all possible responses of the apparatus in its four chosen settings can be specified by means of only four two-valued variables α_1, α_2 and β_1, β_2 . This reduction from eight to four variables depends on the *principle of separability*. In this way, we are led to a situation covered by Theorem 2, and therefore $-2 \leq \langle \gamma \rangle \leq 2$.

By making many measurements for each of the four settings we can determine the four mean values $\langle \alpha_1 \beta_1 \rangle$, $\langle \alpha_1 \beta_2 \rangle$, $\langle \alpha_2 \beta_1 \rangle$, $\langle \alpha_2 \beta_2 \rangle$ and thus the mean value of the correlation

$$\langle \gamma \rangle = \langle \alpha_1 \beta_1 \rangle + \langle \alpha_1 \beta_2 \rangle + \langle \alpha_2 \beta_1 \rangle - \langle \alpha_2 \beta_2 \rangle$$

According to quantum mechanics (which is positivist, probabilistic, and nonseparable), there are cases where the BCHSH inequality is violated. In particular, one can show that for photons in the configuration chosen by Aspect quantum mechanics yields (we will derive this shortly)

$$\langle \gamma \rangle = 3\cos 2\theta - \cos 6\theta \tag{16.58}$$

This leads to values well outside the interval [-2, 2]; for example to $\langle \gamma \rangle = 2\sqrt{2}$ when $\theta = 22.5^{\circ}$ and to $\langle \gamma \rangle = -2\sqrt{2}$ when $\theta = 67.5^{\circ}$.

Proof: The laboratory reference frame Oxyz serves to specify the orientations


Figure 16.20: Detector Orientations

of detectors and polarizers as shown in Figure 16.20 below:

Before any measurements have been made, the photon pair a, b forms a non-separable entity, represented by the vector

$$|\Phi\rangle = \frac{1}{\sqrt{2}} \left(|x_A, x_B\rangle + |y_A, y_B\rangle \right) \tag{16.59}$$

The act of measurement corresponds to passage to the φ -basis. Hence, we require the transition amplitudes from the two states $|x_A, x_B\rangle$, $|y_A, y_B\rangle$ to the four states

$$|\varphi_A,\varphi_B\rangle, |\varphi_A,\varphi_B+\pi/2\rangle, |\varphi_A+\pi/2,\varphi_B\rangle, |\varphi_A+\pi/2,\varphi_B+\pi/2\rangle$$
(16.60)

In the φ -basis we have

$$|\Phi\rangle = \frac{1}{\sqrt{2}} [\cos(\varphi_B - \varphi_A) |\varphi_A, \varphi_B\rangle - \sin(\varphi_B - \varphi_A) |\varphi_A, \varphi_B + \pi/2\rangle + \sin(\varphi_B - \varphi_A) |\varphi_A + \pi/2, \varphi_B\rangle + \cos(\varphi_B - \varphi_A) |\varphi_A + \pi/2, \varphi_B + \pi/2\rangle]$$
(16.61)

The square of each amplitude featured here represents the detection probability. For example, the probability of simultaneously detecting photon a polarized at the angle φ_A and the photon b polarized at the angle φ_B is

$$\left(\frac{1}{\sqrt{2}}\cos(\varphi_B - \varphi_A)\right)^2 = \frac{1}{2}\cos^2(\varphi_B - \varphi_A)$$
(16.62)

By convention, we write the responses of detector A to a photon in state $|\varphi_A\rangle$ (respectively $|\varphi_A + \pi/2\rangle$) as $\alpha = 1$ and similarly with β for detector B.

Let us analyze the four possible responses:

1. $|\varphi_A, \varphi_B\rangle$ gives $\alpha = 1, \beta = 1$ so $\alpha\beta = 1$; the probability is

$$P_{++} = \frac{1}{2}\cos^2(\varphi_B - \varphi_A)$$
 (16.63)

2. $|\varphi_A, \varphi_B + \pi/2\rangle$ gives $\alpha = -1, \beta = 1$ so $\alpha\beta = -1$; the probability is

$$P_{+-} = \frac{1}{2}\sin^2(\varphi_B - \varphi_A)$$
 (16.64)

3. $|\varphi_A + \pi/2, \varphi_B\rangle$ gives $\alpha = 1, \beta = -1$ so $\alpha\beta = -1$; the probability is

$$P_{-+} = \frac{1}{2}\sin^2(\varphi_B - \varphi_A)$$
 (16.65)

4. $|\varphi_A + \pi/2, \varphi_B + \pi/2\rangle$ gives $\alpha = -1, \beta = -1$ so $\alpha\beta = 1$; the probability is

$$P_{--} = \frac{1}{2}\cos^2(\varphi_B - \varphi_A)$$
 (16.66)

The mean value of $\langle \alpha\beta\rangle_{AB}$ follows immediately as

$$(\alpha\beta)_{AB} = P_{++} - P_{+-} - P_{-+} + P_{--} = \cos 2(\varphi_B - \varphi_A)$$
(16.67)

The settings chosen by Aspect are as shown in Figure 16.20 above. Corresponding to it we have the four terms

$$\langle \alpha_1 \beta_1 \rangle = \langle \alpha \beta \rangle_{A_1 B_1} = \cos 2(\varphi_{B_1} - \varphi_{A_1}) = \cos 2\theta \qquad (16.68)$$

$$\langle \alpha_1 \beta_2 \rangle = \langle \alpha \beta \rangle_{A_1 B_2} = \cos 2(\varphi_{B_1} - \varphi_{A_2}) = \cos 2\theta \qquad (16.69)$$

$$\langle \alpha_2 \beta_1 \rangle = \langle \alpha \beta \rangle_{A_2 B_1} = \cos 2(\varphi_{B_2} - \varphi_{A_1}) = \cos 2\theta \tag{16.70}$$

$$\langle \alpha_2 \beta_2 \rangle = \langle \alpha \beta \rangle_{A_2 B_2} = \cos 2(\varphi_{B_2} - \varphi_{A_2}) = \cos 6\theta \tag{16.71}$$

For comparison with Bell's inequality, we introduce the correlation function

$$\langle \gamma \rangle = \langle \alpha_1 \beta_1 \rangle + \langle \alpha_1 \beta_2 \rangle + \langle \alpha_2 \beta_1 \rangle - \langle \alpha_2 \beta_2 \rangle = 3\cos 2\theta - \cos 6\theta \tag{16.72}$$

Thus, the BCHSH test turns the EPR scenario into an arena for rational confrontation between the two interpretations; it remains only to progress from thought experiments to experiments conducted in the laboratory.

16.5.8 The Beginnings of the Experiment at Orsay (1976)

Alain Aspect's experiment studies the correlation between the polarizations of the members of photon pairs emitted by calcium. The light source is a beam of calcium atoms, excited by two focused laser beams having wavelengths $\lambda' = 406 nm$ and $\lambda'' = 581 nm$ respectively. Two-photon excitation produces a state having the quantum number J = 0. When it decays, this state emits two monochromatic photons having the wavelengths $\lambda_1 = 551.3 nm$ and $\lambda_2 =$



Figure 16.21: Calcium based light source - Energy Levels

422.7 nm respectively, in a cascade of two electronic transitions from the initial J = 0 level to the final J = 0 state, passing through an intermediate J = 1 state, as shown in Figure 16.21 below which shows the excitation and decay of the calcium atom.

The mean lifetime of the intermediate state is 4.7 ns. To simplify the terminology, we shall call the $\lambda_1 = 551.3 nm$ light green, and the $\lambda_2 = 422.7 nm$ light violet.

The polarizer, which works like a Wollaston prism is shown in Figure 16.22 below where we can see the two-valued response of a Wollaston prism.



Figure 16.22: Wollason Prism - Polarizer

The Wollaston prism is made of quartz or of calcite. It splits an incident beam of natural (unpolarized) light into two beams of equal intensity, polarized at 90° to each other. If only a single unpolarized photon is incident, it emerges either in the state $|x\rangle$, with probability 1/2, or in the state $|y\rangle$, with probability 1/2. Thus, the response of the system is two-valued.

The photon is detected by the photomultiplier tubes (PM) downstream from the prism. Every electric pulse from these detectors corresponds to the passage of a photon, allowing the photons to be counted. The experimental layout is sketched in Figure 16.23 below, which shows a sketch of the first Orsay experiment.



Figure 16.23: First Orsay Experiment

? It uses a coincidence circuit which registers an event whenever two photons are detected in cascade. In this way four separate counts are recorded simultaneously, over some given period of time. In the EPR scenario envisaged by Bohm, where $\theta = 0$, the only possible responses are (+1, -1) or (-1, +1) In the situation realized by Aspect, the angle θ is non-zero, and four different responses are possible.

- 1. N_{++} the number of coincidences corresponding to α = 1 and β = 1, that is, to $\alpha\beta$ = 1
- 2. N_{+-} the number of coincidences corresponding to $\alpha = 1$ and $\beta = -1$, that is, to $\alpha\beta = -1$
- 3. N_{-+} the number of coincidences corresponding to $\alpha=-1$ and $\beta=1,$ that is, to $\alpha\beta=-1$
- 4. N_{--} the number of coincidences corresponding to α = –1 and β = –1, that is, to $\alpha\beta$ = 1

The resolving time of the coincidence circuit is 10 ns, meaning that it reckons two photons as coincident if the they are separated in time by no more than 10 ns. The mean life of the intermediate state of the calcium atom is 4.7 ns. Therefore, after a lapse of 10 ns, that is more than twice the mean lifetime, almost all the atoms have decayed (actually 88%). In other words, the efficiency of the coincidence counter is very high.

The experiment consists in counting, over some given time interval, the four kinds of coincidence: N_{++}, N_{+-}, N_{-+} and N_{--} . The total number of events is $N = N_{++} + N_{+-} + N_{-+} + N_{--}$.

Accordingly, the different kinds of coincidence have probabilities

$$\begin{aligned} P_{++} &= N_{++}/N \text{ corresponding to } \alpha\beta = 1 \\ P_{+-} &= N_{+-}/N \text{ corresponding to } \alpha\beta = -1 \\ P_{-+} &= N_{-+}/N \text{ corresponding to } \alpha\beta = -1 \\ P_{--} &= N_{--}/N \text{ corresponding to } \alpha\beta = 1 \end{aligned}$$

and the measured average of $\alpha\beta$ is

$$\langle \alpha \beta \rangle = \frac{N_{++} - N_{+-} - N_{-+} + N_{--}}{N} \tag{16.73}$$

Each set of four coincidence counts corresponds to one particular setting of (\vec{A}, \vec{B}) , and yields a mean value $\langle \alpha \beta \rangle$. But in order to determine the correlation function $\langle \gamma \rangle$ used in the BCHSH inequality, we need four mean values $\langle \alpha \beta \rangle$. Therefore, we choose, in succession four different settings as shown in Figure 16.18(c); four counting runs then yield the four mean values $\langle \alpha_1 \beta_1 \rangle$, $\langle \alpha_1 \beta_2 \rangle$, $\langle \alpha_2 \beta_1 \rangle$, $\langle \alpha_2 \beta_2 \rangle$ which then determine the value of $\langle \gamma \rangle$ via

$$\langle \gamma \rangle = \langle \alpha_1 \beta_1 \rangle + \langle \alpha_1 \beta_2 \rangle + \langle \alpha_2 \beta_1 \rangle - \langle \alpha_2 \beta_2 \rangle \tag{16.74}$$

The Results of the First Experiment at Orsay

The results of the first Orsay experiment are shown in Figure 16.24 below. The angle θ which specifies the setting of the polarizers is plotted horizontally, and the mean value $\langle \gamma \rangle$ vertically.



Figure 16.24: Results from First Orsay Experiment

From earlier, the correlation function predicted by quantum mechanics reads

$$\langle \gamma \rangle = 3\cos 2\theta - \cos 6\theta \tag{16.75}$$

It is drawn as the solid curve on the graph (the curve has been corrected for instrumental effects, which explains why its ends are not precisely at 2 and -2). According to the BCHSH inequality

$$-2 \le \langle \gamma \rangle \le 2 \tag{16.76}$$

so that hidden-variable theories exclude the cross-hatched regions of the plane, which correspond to $\langle \gamma \rangle > 2$ or $\langle \gamma \rangle < -2$.

The experimental results from 17 different values of θ are indicated on the figure by squares, where the vertical size of the square gives plus or minus one standard deviation (a measure of the experimental error).

Clearly, there can be no doubt that the BCHSH inequality is violated; many of the experimental points fall outside the interval [-2, 2]. At the point where the violation is maximal ($\theta = 22.5^{\circ}$), one finds

$$\langle \gamma \rangle = 2.70 \pm 0.015$$
 (16.77)

which represents a departure of over 40 standard deviations from the extreme value of 2. What is even more convincing is the precision with which the experimental points lie on the curve predicted by quantum mechanics.

Quite evidently, for the EPR scenario one must conclude not only that hiddenvariable theories fail, but also that quantum mechanics is positively the right theory for describing the observations.

The Relativistic Test

The EPR experiment just described shows that the measurements in A and B are correlated. What is the origin of the correlations?

According to quantum theory, before the measurement each particle pair constitutes a single system extending from A to B, whose two parts are non-separable and correlated. This interpretation corresponds to a violation of Bell's inequality and agreement with experiment.

According to hidden-variables theories, the particle pair is characterized, at the instant of decay, by its hidden variable, which determines the correlation between the polarizations measured in A and B. This interpretation satisfies Bell's inequality but disagrees with experiment.

Accordingly, the Orsay experiment supports the quantum interpretation (in

terms of the correlation between two parts A and B of a single system).

However, to clinch this conclusion, one must ensure that no influence is exerted in the ordinary classical sense through some interaction propagated between the two detectors A and B, that is, no influence which might take effect after the decay at S, and which might be responsible for the correlation actually observed.

Let us therefore examine the Orsay apparatus in more detail as in Figure 16.25 below where we attempt to test Einsteinian non-separability.



Figure 16.25: Orsay Experiment - Details

When the detectors at A and B record a coincidence, this means that both have been triggered within a time interval of at most 10 ns, the resolving time of the circuit. Could it happen that, within this interval, A sends to B a signal capable of influencing the response of B? In the most favorable case, such a signal would travel with the speed of light in vacuum, which according to relativity theory is the upper limit on the propagation speed of information, and thereby of energy. To cover the distance AB, which is 12 m in the figure, such a signal would need 40 ns. This is too long by at least 30 ns, and rules out any causal links between A and B in the sense of classical physics. One says that the interval between A and B is space-like.

One of the advantages of the Orsay experiment is that it uses a very strong light-source, allowing sufficient distance between the detectors A and B while still preserving reasonable counting rates. By increasing the distance AB step by step, Aspect could check that the correlation persists, even when the interval between A and B becomes space-like. This is the check that guarantees that the two-photon system is non-separable irrespective of the distance AB.

It has become the custom to speak of the principle of Einsteinian separability in order to denote the absence of correlations between two events separated by a space-like interval. This is the principle that the Orsay experiment invites us to reconsider, even though our minds, used to the world at the macroscopic level, find it difficult to conceive of two *microscopic* photons 12m apart as a single indivisible object.

The Final Stage of the Experiment at Orsay (1983)

Though the results of the first Orsay experiment are unarguable and clear-cut, the conclusion they invite is so startling that one should not be surprised at the appearance of a last-ditch objection, which as it happens gave the experimenters a great deal of trouble. In the preceding section we discussed the possible role of interactions between A and B operating after the decay at S, and duly eliminated the objection. But one can also ask whether correlations might be introduced through an interaction operating before the decay. We could imagine that the decay itself is preconditioned by the setting of detectors A and B, such influences taking effect through the exchange of signals between the detectors and the source. No such mechanism is known a priori, but we do know that, if there is one, then Einsteinian non-separability would cease to be a problem, because the mechanism could come into action long before the decay, removing any reason for expecting a minimum 30 ns delay. Though such a scenario is very unlikely, the objection is a serious one and must be taken into account; to get around it, the experimenter must be able to choose the orientation of the detectors A and B at random after the decay has happened at S. In more picturesque language, we would say that the two photons must leave the source without knowing the orientations of the polarizers A and B. Briefly put, this means that it must be possible to change the detector orientations during the 20 ns transits over SA and SB.

The solution adopted at Orsay employs periodic switching every 10 ns. These changes are governed by two independent oscillators, one for channel A and one for channel B. The oscillators are stabilized, but however good the stabilization it cannot eliminate small random drifts that are different in the two channels, seeing that the oscillators are independent. This ensures that the changes of orientation are random even though the oscillations are periodic, provided the experiment lasts long enough (1 to 3 hours).

The key element of the second Orsay experiment is the optical switch shown in Figure 16.26 below.



Figure 16.26: Second Orsay Experiment - Optical Switch

In a water tank, a system of standing waves is produced by electro-acoustic excitation at a frequency of 25 MHz (corresponds to 10 ns between switchings).

The fluid keeps changing from a state of perfect rest to one of maximum agitation and back again. In the state of rest, the light beam is simply transmitted, In the state of maximum agitation, the fluid arranges itself into a structure of parallel and equidistant plane layers, alternately stationary (nodal planes) or agitated (antinodal planes). Thus, one sets up a lattice of net-like diffracting planes; the diffracted intensity is maximum at the so-called Bragg angles, just as in scattering from a crystal lattice. Here the light beam is deviated through 10^2 radians (the angles in the figure are exaggerated for effect). The two numerical values, 25 MHz and 10^2 radians, suffice to show the magnitude of the technical achievement. With the acoustic power of 1 watt, the system functions as an ideally efficient switch.

The second Orsay experiment (using optical switches) is sketched in Figure 16.27 below.



Figure 16.27: Second Orsay Experiment using Optical Switches

In this set-up, the photons a and b leave S without *knowing* whether they will go, the first to A_1 or A_2 and the second to B_1 or B_2 .

The second experiment is less precise than the first, because the light beams must be very highly collimated in order to ensure efficient switching. Nevertheless, its results exhibit an unambiguous violation of Bell's inequality, reaching 5 standard deviations at the peak; moreover the results are entirely compatible with the predictions of quantum mechanics.

16.6 The Principle of Non-Separability

Experiment has spoken. Half a century after the Como conference, Bohr's interpretation once again beats Einstein's, in a debate more subtle and also more searching. There were two conflicting theories:

| Einstein | Bohr | |
|------------------|-------------------|--|
| hidden variables | quantum mechanics | |
| realist | positivist | |
| deterministic | probabilistic | |
| separable | non-separable | |

Table 16.2: Two Conflicting Theories

The violation of the BCHSH inequality argues for Bohr's interpretation, all the more so as the measured values of $\langle \gamma \rangle$ are in close agreement with the predictions of quantum mechanics.

It remains to ask oneself just why hidden-variable theories do fail. Of the three basic assumptions adopted by such theories, namely realism, determinism, and separability, at least one must be abandoned. In the last resort, it is separability that seems to be the most vulnerable assumption. Indeed, one observes experimentally that the violation of the BCHSH inequality is independent of the distance between the two detectors A and B, even when this distance is 12 m or more. There are still die-hard advocates of determinism, who try to explain non-separability through non-local hidden variables. Such theories, awkward and barely predictive, are typically ad hoc, and fit only a limited number of phenomena. They are weakly placed to defend themselves against interpretations furnished by quantum mechanics, which have the virtues of simplicity, elegance, efficiency, and generality, and which are invariably confirmed by experiment.

The principle of Einsteinian separability asserts that there are no correlations between two phenomena separated by a space-like interval. In other words, no interaction can propagate faster than light in vacuum. In an EPR scenario this principle must be abandoned, and replaced by a principle asserting nonseparability: in a quantum system evolving free of external perturbations, and from well-defined initial conditions, all parts of the system remain correlated, even when the interval between them is space-like

This assertion reflects the properties of the state vector of a quantum system. For an EPR system, the state vector after the decay of the source reads

$$|\Phi\rangle = \frac{1}{\sqrt{2}} \left(|x_A, x_B\rangle + |y_A, y_B\rangle \right) \tag{16.78}$$

This expression combines the elements A and B in a non-separable manner, which is what explains the observed correlations. The truth is that all this has been well known ever since the beginnings of quantum mechanics, with the concept of the electron cloud as the most telling illustration. It is for instance hard to imagine separability between the 92 electrons of a uranium atom. What is new is that quantum mechanics, considered hitherto as a microscopic theory applicable on the atomic scale, is now seen to apply to a two-particle system macroscopically, on the scale of meters. The truly original achievement of Aspect's experiment is the demonstration of this fact.

Quantum objects have by no means exhausted their capacity to astonish us by their difference from the properties of the macroscopic objects in our everyday surroundings. In the preceding sections we saw that a photon can interfere with itself and we have shown that two photons 12m apart constitute but a single object. Thus, it becomes ever more difficult to picture a photon through analogies with rifle bullets, surface waves in water, clouds in the sky, or with any other object of our familiar universe. Such partial analogies fail under attempts to make them more complete, and through their failure we discover new properties pertaining to quantum objects. The only fruitful procedure is to follow the advice of Niels Bohr, namely, to bend one's mind to the new quantum concepts until they become habitual and thereby intuitive. Earlier generations of physicists have had to face similar problems. They had to progress from Aristotle's mechanics to Newton's, and then from Newton's to Einstein's. The same effort is now required of us, at a time favorable in that, by mastering the EPR paradox, quantum mechanics has passed a particularly severe test with flying colors.

From this point of view, the principle of non-separability seems as important as the principle of special relativity, and Aspect's experiment plays the same role now that the Michelson-Morley experiment played then.

16.7 An Example and a Solution - Bell's Theorem with Photons

Two photons fly apart from one another, and are in oppositely oriented circularly polarized states. One strikes a polaroid film with axis parallel to the unit vector \hat{a} , the other a polaroid with axis parallel to the unit vector \hat{b} . Let $P_{++}(\hat{a},\hat{b})$ be the joint probability that both photons are transmitted through their respective polaroids. Similarly, $P_{--}(\hat{a},\hat{b})$ is the probability that both photons are absorbed by their respective polaroids, $P_{+-}(\hat{a},\hat{b})$ is the probability that the photon at the \hat{a} polaroid is transmitted and the other is absorbed, and finally, $P_{-+}(\hat{a},\hat{b})$ is the probability that the photon at the \hat{a} polaroid is absorbed and the other is transmitted.

The classical realist assumption is that these probabilities can be separated:

$$P_{ij}(\hat{a},\hat{b}) = \int d\lambda \,\rho(\lambda) P_i(\hat{a},\lambda) P_j(\hat{b},\lambda) \tag{16.79}$$

where *i* and *j* take on the values + and –, where λ signifies the so-called hidden variables, and where $\rho(\lambda)$ is a weight function. This equation is called the separable form.

The correlation coefficient is defined by

$$C(\hat{a},\hat{b}) = P_{++}(\hat{a},\hat{b}) + P_{--}(\hat{a},\hat{b}) - P_{+-}(\hat{a},\hat{b}) - P_{-+}(\hat{a},\hat{b})$$
(16.80)

and so we can write

$$C(\hat{a},\hat{b}) = \int d\lambda \,\rho(\lambda) C(\hat{a},\lambda) C(\hat{b},\lambda)$$
(16.81)

where

$$C(\hat{a},\lambda) = P_+(\hat{a},\lambda) - P_-(\hat{a},\lambda)$$
(16.82)

$$C(\hat{b},\lambda) = P_+(\hat{b},\lambda) - P_-(\hat{b},\lambda)$$
(16.83)

It is required that

(a) $\rho(\lambda) \ge 0$ (b) $\int d\lambda \,\rho(\lambda) = 1$ (c) $-1 \le C(\hat{a}, \lambda) \le 1$, $-1 \le C(\hat{b}, \lambda) \le 1$

The Bell coefficient

$$B = C(\hat{a}, \hat{b}) + C(\hat{a}, \hat{b}') + C(\hat{a}', \hat{b}) - C(\hat{a}', \hat{b}')$$
(16.84)

combines four different combinations of the polaroid directions.

- (1) Show that the above classical realist assumptions imply that $|B| \leq 2$.
- (2) Show that quantum mechanics predicts that $C(\hat{a}, \hat{b}) = 2(\hat{a} \cdot \hat{b})^2 1$.
- (3) Show that the maximum value of the Bell coefficient is $2\sqrt{2}$, according to quantum mechanics.
- (4) Cast the quantum mechanical expression for $C(\hat{a}, \hat{b})$ into a separable form. Which of the classical requirements, (a), (b), or (c) above is violated?

Solution

(1) With the separability assumption, we have (16.81)

$$C(\hat{a},\hat{b}) = \int d\lambda \,\rho(\lambda) C(\hat{a},\lambda) C(\hat{b},\lambda)$$

It follows that the Bell coefficient can be written in the form

$$B = C(\hat{a}, \hat{b}) + C(\hat{a}, \hat{b}') + C(\hat{a}', \hat{b}) - C(\hat{a}', \hat{b}')$$

=
$$\int d\lambda \rho(\lambda) [C(\hat{a}, \lambda) (C(\hat{b}, \lambda) + C(\hat{b}', \lambda)) + C(\hat{a}', \lambda) (C(\hat{b}, \lambda) - C(\hat{b}', \lambda))]$$
(16.85)

Since $|C(\hat{a}, \lambda)| \leq 1$, $|C(\hat{a}', \lambda)| \leq 1$ and $\rho(\lambda) \geq 0$, we have

$$|B| \leq \int d\lambda \rho(\lambda) \left(\left| C(\hat{b}, \lambda) + C(\hat{b}', \lambda) \right| + \left| C(\hat{b}, \lambda) - C(\hat{b}', \lambda) \right| \right)$$
(16.86)

Now suppose that for a given λ , $C_M(\lambda)$ is the maximum and $C_m(\lambda)$ is the minimum of $C(\hat{b}, \lambda)$ and $C(\hat{b}', \lambda)$, so that $C_M(\lambda) \ge C_m(\lambda)$. Then

$$|B| \leq \int d\lambda \rho(\lambda) \left(|C_M(\lambda) + C_m(\lambda)| + C_M(\lambda) - C_m(\lambda) \right)$$
(16.87)

There are two cases to consider.

For the case $C_M(\lambda) \ge 0$, we have $|C_M(\lambda) + C_m(\lambda)| = C_M(\lambda) + C_m(\lambda)$ so that

$$|B| \leq \int d\lambda \rho(\lambda) \left(C_M(\lambda) + C_m(\lambda) + C_M(\lambda) - C_m(\lambda) \right)$$

= $2 \int d\lambda \rho(\lambda) C_M(\lambda) \leq 2 \int d\lambda \rho(\lambda) |C_M(\lambda)| \leq 2 \int d\lambda \rho(\lambda) = 2$

For the case $C_M(\lambda) < 0$, we have $|C_M(\lambda) + C_m(\lambda)| = -C_M(\lambda) - C_m(\lambda)$ so that

$$|B| \leq \int d\lambda \rho(\lambda) \left(-C_M(\lambda) - C_m(\lambda) + C_M(\lambda) - C_m(\lambda) \right)$$

= $2 \int d\lambda \rho(\lambda) \left(-C_m(\lambda) \right) \leq 2 \int d\lambda \rho(\lambda) |C_m(\lambda)| \leq 2 \int d\lambda \rho(\lambda) = 2$

Thus, in all cases $|B| \leq 2$.

(2) A photon, traveling in the y-direction, might have right- or left-handed circular polarization. The corresponding quantum states are written $|R\rangle$ and $|L\rangle$ respectively. These circular polarization states can be expressed as coherent superpositions of linearly polarized states in the z and x directions:

$$|R\rangle = \frac{1}{\sqrt{2}} \left(|z\rangle + i |x\rangle\right) \quad , \quad |L\rangle = \frac{1}{\sqrt{2}} \left(|z\rangle - i |x\rangle\right) \tag{16.88}$$

Under a rotation of the coordinate axes by an angle θ about the y direction, $|R\rangle \rightarrow e^{i\theta} |R\rangle$ and $|L\rangle \rightarrow e^{-i\theta} |L\rangle$ or equivalently

$$\begin{pmatrix} |z\rangle\\|x\rangle \end{pmatrix} \rightarrow \begin{pmatrix} |z'\rangle\\|x'\rangle \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta\\\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} |z\rangle\\|x\rangle \end{pmatrix}$$
(16.89)

If each photon is in a state of right-handed circular polarization, we write the corresponding state vector as $|R_1\rangle |R_2\rangle$. However, since the photons are moving in opposite directions, one along the positive, and the other along the negative y axis, it follows that the actual directions in which the electric fields rotate, in time, in the vicinity of the two photons, are opposed to one another. The same holds for the state $|L_1\rangle |L_2\rangle$, corresponding to each photon being in a state of left-handed circular polarization.

The linear combination of these two states,

$$|EPR\rangle = \frac{1}{\sqrt{2}} \left(|R_1\rangle |R_2\rangle + |L_1\rangle |L_2\rangle \right) \tag{16.90}$$

corresponds to the more general situation in which the photons are in oppositely oriented states of circular polarization, where the sense of this polarization is not specified. We can write this *entangled* or *Einstein-Podolsky-Rosen* state in the form

$$|EPR\rangle = \frac{1}{\sqrt{2}} \left(|z_1\rangle |z_2\rangle - |x_1\rangle |x_2\rangle \right) \tag{16.91}$$

which is a superposition of states of linear polarization.

Suppose now that a measurement of linear polarization is made on photon 1 in the z direction, and of photon 2 in the z' direction, that is, the z direction after a rotation of the axes about the y axis. The probability amplitude associated with this measurement on the EPR state is

$$\langle EPR \mid z_1 z_2' \rangle = \frac{1}{\sqrt{2}} \left(\langle z_1 \mid \langle z_2 \mid - \langle x_1 \mid \langle x_2 \mid \rangle \left(|z_1 \rangle \left(\cos \theta \mid z_2 \right) - \sin \theta \mid x_2 \right) \right) \right)$$
$$= \frac{1}{\sqrt{2}} \cos \theta \tag{16.92}$$

where we have used $\langle z_1 | x_1 \rangle = 0$. The probability that photon 1 is found to have linear polarization in the direction z, and photon 2 in the direction z' is

$$P_{++}(\hat{a},\hat{b}) = |\langle EPR \mid z_1 z_2' \rangle|^2 = \frac{1}{2} \cos^2 \theta$$
 (16.93)

where we have assumed that \hat{a} is in the z direction and \hat{b} is in the z' direction.

Suppose next that the linear polarization of the linear polarization of photon 1 were measured in the x direction, and that of photon 2 again in the z' direction. The probability amplitude is

$$\langle EPR \mid x_1 z_2' \rangle = \frac{1}{\sqrt{2}} \left(\langle z_1 \mid \langle z_2 \mid - \langle x_1 \mid \langle x_2 \mid \rangle \left(|x_1\rangle \left(\cos \theta \mid z_2 \right) - \sin \theta \mid x_2 \right) \right) \right)$$
$$= \frac{1}{\sqrt{2}} \sin \theta \tag{16.94}$$

If photon 1 has polarization in the x direction, then it will not be transmitted by a polarizer in the z direction - it will be absorbed. Hence,

$$P_{-+}(\hat{a},\hat{b}) = |\langle EPR \mid x_1 z_2' \rangle|^2 = \frac{1}{2} \sin^2 \theta$$
 (16.95)

Similarly,

$$P_{+-}(\hat{a},\hat{b}) = \left| \left\langle EPR \mid z_1 x_2' \right\rangle \right|^2 = \frac{1}{2} \sin^2 \theta \tag{16.96}$$

$$P_{--}(\hat{a},\hat{b}) = |\langle EPR \mid x_1 x_2' \rangle|^2 = \frac{1}{2} \cos^2 \theta$$
 (16.97)

The correlation coefficient is then

$$C(\hat{a},\hat{b}) = P_{++}(\hat{a},\hat{b}) + P_{--}(\hat{a},\hat{b}) - P_{+-}(\hat{a},\hat{b}) - P_{-+}(\hat{a},\hat{b})$$

= $\cos^2\theta - \sin^2\theta = 2\cos^2\theta - 1 = \cos 2\theta$ (16.98)

Since the unit vectors \hat{a} and \hat{b} are at an angle θ with respect to one another, it follows that $\hat{a} \cdot \hat{b} = \cos \theta$ and therefore

$$C(\hat{a},\hat{b}) = 2\cos^2\theta - 1 = 2(\hat{a}\cdot\hat{b})^2 - 1$$
(16.99)

(3) Suppose that the angle between the vectors \hat{a}' and \hat{a} is x/2, between \hat{a} and \hat{b} is y/2 and between \hat{b} and \hat{b}' is z/2. Then the angle between \hat{a}' and \hat{b}' is (x + y + z)/2 and according to quantum mechanics, the Bell coefficient has the form

$$B = \cos x + \cos y + \cos z - \cos(x + y + z)$$
(16.100)

This function has extrema when

$$\frac{\partial B}{\partial x} = -\sin x + \sin(x + y + z) = 0$$
$$\frac{\partial B}{\partial y} = -\sin y + \sin(x + y + z) = 0$$
$$\frac{\partial B}{\partial z} = -\sin z + \sin(x + y + z) = 0$$

$$\sin x = \sin y = \sin z = \sin(x + y + z)$$
 (16.101)

This has the solution

$$x = y = z \text{ and } 3x = \pi - x \to x = \pi/4$$
 (16.102)

For this extremum

$$B = 3\cos\frac{\pi}{4} - \cos\frac{3\pi}{4} = \frac{3}{\sqrt{2}} + \frac{1}{\sqrt{2}} = 2\sqrt{2}$$
(16.103)

This is a maximum, since at this point

$$\frac{\partial^2 B}{\partial x^2} = \frac{\partial^2 B}{\partial y^2} = \frac{\partial^2 B}{\partial z^2} = -\cos\frac{\pi}{4} + \cos\frac{3\pi}{4} = -\sqrt{2} < 0$$

(4) Let the vector \hat{a} be at an angle θ_a with respect to some direction in the xz plane, and let \hat{b} be at an angle θ_b with respect to the same direction. Then

$$C(\hat{a}, b) = \cos 2(\theta_a - \theta_b)$$

= $\cos 2\theta_a \cos 2\theta_b + \sin 2\theta_a \sin 2\theta_b$
= $\int d\lambda \rho(\lambda) C(\hat{a}, \lambda) C(\hat{b}, \lambda)$ (16.104)

and with the assignments

$$\rho(\lambda) = \delta(\lambda + 1) + \delta(\lambda - 1)$$

$$C(\hat{a}, 1) = \cos 2\theta_a \quad , \quad C(\hat{a}, -1) = \sin 2\theta_a$$

$$C(\hat{b}, 1) = \cos 2\theta_b \quad , \quad C(\hat{b}, -1) = \sin 2\theta_b$$

we then see that

$$\rho(\lambda) \ge 0$$

-1 \le C(\hat{a}, \lambda), C(\hat{b}, \lambda) \le 1 for \lambda = \pm 1

but

$$\int d\lambda \, \rho(\lambda) = 1 + 1 = 2$$

so that the normalization condition (b) is violated.

16.8 Non-Locality, EPR and Bell - a last time

As we discussed earlier, the second major problem confronting hidden variables and possessed properties was first understood in the context of the EPR paradox and then reinforced by the Bell inequalities. Let us look back at these ideas in light of the above discussions.

or

The original EPR analysis was rather complex in a technical sense and most discussions now use a simpler version due to Bohm. He considered a particle whose decay produces two spin-1/2 particles whose total spin angular momentum is zero. These particles move away from each other in opposite directions, and the components of their spins along various directions are subsequently measured by two observers, N and L, say. The constraint on the total spin means that if both observers agree to measure the spin along a certain direction \hat{n} , and if N measures $+\hbar/2$, then L will necessarily get the result $-\hbar/2$, and if N measures $-\hbar/2$, then L will necessarily get the result $+\hbar/2$.

There are no surprises if such correlations are analyzed in the context of classical physics. If one particle emerges from the decay with its internal angular momentum vector pointing along some particular direction, then because of conservation of angular momentum, the second particle is guaranteed to emerge with its spin vector pointing in the opposite direction. Thus, the 100% anticorrelations found in the measurements made by the two observers are simply the result of the fact that both particles possess actual, and (anti-)correlated, values of internal angular momentum and this is true from the time they emerge from the decay to the time the measurements are made. There are no paradoxes here, and everything is in accord with the simple realist view of classical physics.

The situation in quantum theory is radically different. Suppose first that the measurements are made along the z-axes of the two observers. The spin part of the state of the two particles can be written in terms of the associated eigenvectors as

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle |\downarrow\rangle - |\downarrow\rangle |\uparrow\rangle\right) \tag{16.105}$$

where, for example, $|\uparrow\rangle|\downarrow\rangle$ is the state in which particles 1 and 2 have spin $+\hbar/2$ and $-\hbar/2$ respectively. Thus

$$\hat{S}_{z}|\uparrow\rangle = +\hbar/2|\uparrow\rangle$$
, $\hat{S}_{z}|\downarrow\rangle = -\hbar/2|\downarrow\rangle$ (16.106)

The pragmatic or instrumentalist interpretation of the entangled state $|\psi\rangle$ is straightforward. If, in a series of repeated measurements by N, a selection is made of the pairs of particles for which the measurement of particle gave spinup, then - with probability one - a series of measurements by L on her particle in these pairs will yield spin-down. Similarly, if N finds spin-down then, with probability one, L will find spin-up. This correlation can be explained by saying that the measurements by N(computed with the operator $\hat{S}_z \otimes \hat{I}$) **cause** a reduction of the state vector from $|\psi\rangle$ to $|\uparrow\rangle|\downarrow\rangle$ or $|\downarrow\rangle|\uparrow\rangle$ respectively according to whether the spin-up or the spin-down result is selected. This new state is an eigenstate of the operator $\hat{I} \otimes \hat{S}_z$ associated with the second particle, and with an eigenvalue that is the opposite of the result obtained by N.

This description is acceptable within the confines of the pragmatic approach to quantum theory, but difficulties arise if one tries to enforce a more realist interpretation of the above entangled state.

The obvious question is how the information about each observer's individual results *gets to* the other particle to guarantee that the result obtained by the second observer will be the correct one.

One might be tempted to invoke the reasoning of classical physics and argue that both particles *possess* the appropriate value all the time.

However, the only way in standard quantum theory of guaranteeing that a certain result will be obtained is if the state is an eigenvector of the observable concerned. But the state $|\psi\rangle$ above is *not* of this type. In fact, it displays the typical features of quantum entanglement - it is a superposition of states. Any attempt to invoke a hidden variable resolution will have to cope with the implications of the Kochen-Specker theorem.

There is also a question of whether this picture is compatible with special relativity. If the measurements by the two observers are space-like separated (which can be easily arranged) then which of them makes the first measurement and hence, in the standard interpretation, causes the state-vector reduction is clearly reference-frame dependent.

The problem is compounded by considering what happens if the observers decide to measure, say, the x-component of the spins, rather than the z-components. The state above can now be written in terms of \hat{S}_x eigenvectors as

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\langle +\rangle\rangle | \rightarrow\rangle - |\rightarrow\rangle\rangle |\langle -\rangle\rangle\right) \tag{16.107}$$

where $| \rightarrow \rangle$ and $| \leftarrow \rangle$ correspond to eigenvalues $+\hbar/2$ and $-\hbar/2$ respectively of the operator \hat{S}_x .

In one sense, this new entangled state is what might have been expected, and confirms that there is the same type of 100% anti-correlation between \hat{S}_x measurements as that found for the observable \hat{S}_z . Indeed, this argument can be generalized to show that for any unit vector \hat{n} , the entangled state can be rewritten as a sum of two anti-correlated terms containing eigenvectors of the projection $\hat{n} \cdot \hat{S}$ of the spin operator along \hat{n} . Thus, if one adopts the classical type argument, one is obliged to conclude that both particles possessed exact values of spin along any axis from the moment they left the decay. This might not be easy to reconcile with the uncertainty relations associated with the angular momentum commutators.

EPR considered these issues, and concluded that the difficulties could be resolved in one of only two ways:

1. When N makes her measurement, the result communicates itself at once

in some way to particle 2, and converts its state into the appropriate eigenvector.

or

2. Quantum theory is incomplete and provides only a partial specification of the actual state of the system.

In contemplating the first possibility it must be appreciated that the two particles may have moved a vast distance apart before the first measurement is made and, therefore, any *at once* mode of communication would be in violent contradiction with the spirit (if not the law) of special relativity. It is not surprising that Einstein was not very keen on this alternative! An additional objection involves the lack within quantum theory itself of any idea about how this non-local effect is supposed to take place, so in this sense the theory would be incomplete anyway.

EPR came to the conclusion that the theory is indeed incomplete, although they left open the correct way in to *complete* it. One natural path is to suppose that there exist *hidden variables* whose values are not accessible to measurement in the normal way but which determine the actual values of what we normally regard as observables - in the same way as do the microstates in classical statistical physics.

However, it is not a trivial matter to construct a hidden variable theory that reproduces all of the empirical results of quantum mechanics (which are experimentally correct!). In particular, such a theory would need to explain why it is that certain observables are incompatible (those with non-vanishing commutator) in the sense that one cannot prepare a state of the system that violates the predictions of the uncertainty relations. In addition, there is the need to come to terms with the implications of the Kochen-Specker theorem.

Hidden variable theories capable of reproducing the results of conventional quantum theory do in fact exist (Bohm for example) but they exhibit a non-locality which is every bit as peculiar as that discussed above. One might think that this is a deficiency of these particular theories and that others might exist without this problem.

However, as we discussed earlier and will review here again, a very famous result of John Bell shows that this is not possible, that is, any hidden-variable theory that exactly replicates the results of quantum theory will necessarily possess striking non-local features.

This result is of major importance in understanding and appreciating the conceptual challenge posed by quantum theory.

16.8.1 The Bell Inequalities

As with the Kochen-Specker result, the non-locality property we are about to discuss is not just a feature of hidden variables theories. It applies to *any* realist interpretation of quantum theory in which it is deemed meaningful to say that an individual system *possesses* values for its physical quantities in a way that is analogous to that in classical physics.

We will derive an inequality that is satisfied by certain correlation functions in any such theory *which is also local*. We will then see that the predictions (which are experimentally correct) of quantum theory violate this inequality.

The considerations of EPR were concerned with two observers who make measurements along the same axis. Bell found his famous inequalities by asking what happens if the observers measure the spin of the particles along different axes. In particular, we consider a pair of unit vectors \hat{a} and \hat{a}' for one observer and another pair \hat{b} and \hat{b}' for the other observer.

Now suppose a series of repeated measurements is made on a collection of systems whose quantum state is described by the entangled state vector $|\psi\rangle$. For example, we could look at a series of decays, each of which produces a pair of particles with zero total spin angular momentum. The central realist assumption we are testing is that each particle has a definite value at all times for any direction of spin. We let a_n denote $2/\hbar$ times the value of $\hat{a} \cdot \hat{S}$ possessed by particle 1 in the n^{th} element of the collection. Thus $a_n = \pm 1$ if $\hat{a} \cdot \hat{S} = \pm \hbar/2$.

The key ingredient in the derivation of the Bell inequalities is the correlation between measurements made by the two observers along these different directions. For directions \hat{a} and \hat{b} this is defined by

$$C(\hat{a}, \hat{b}) \coloneqq \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} a_n b_n$$
 (16.108)

and similarly for the other directions. Note that if the results are always totally correlated (spins always in the same direction) then $C(\hat{a}, \hat{b}) = +1$, whereas if they are totally anti-correlated (spins always in opposite directions) we get $C(\hat{a}, \hat{b}) = -1$.

Now look at the quantity

$$g_n \coloneqq a_n b_n + a_n b'_n + a'_n b_n + a'_n b'_n \tag{16.109}$$

For any member n of the collection, each term in this sum will take on the value +1 or -1. Furthermore, the fourth term on the right hand side is equal to the product of the first three (because $(a_n)^2 = 1 = (b_n)^2$). Then thinking about the various possibilities shows that g_n can take on only the values ± 2 . Therefore,

the right hand side of the expression

$$\left|\frac{1}{N}\sum_{n=1}^{N}g_{n}\right| = \left|\frac{1}{N}\sum_{n=1}^{N}a_{n}b_{n} + \frac{1}{N}\sum_{n=1}^{N}a_{n}b_{n}' + \frac{1}{N}\sum_{n=1}^{N}a_{n}'b_{n} - \frac{1}{N}\sum_{n=1}^{N}a_{n}'b_{n}'\right|$$

representing the average value of g_n must be less than or equal to 2. Thus in the limit as $N \to \infty$, we get

$$\left| C(\hat{a}, \hat{b}) + C(\hat{a}, \hat{b}') + C(\hat{a}', \hat{b}) - C(\hat{a}', \hat{b}') \right| \le 2$$
(16.110)

which is one of the famous Bell inequalities.

It is important to emphasize the only assumptions that have gone into proving this inequality are:

- 1. For each particle it is meaningful to talk about the actual values of the projection of the spin along any direction.
- 2. There is locality in the sense that the value of any physical quantity is not changed by altering the position of a remote piece of measuring equipment.

This means that both occurrences of a_n in the expression for the average value of g_n have the same value, that is, they do not depend on the direction $(\hat{b} \text{ or } \hat{b}')$ along which the other observer chooses to measure the spin of particle 2. In particular, we are ruling out the type of context-dependent values that arose in our discussion of the Kochen-Specker theorem.

We will now show that the predictions of quantum theory violate this inequality over a range of directions for the spin measurements. The quantum mechanical prediction for the correlation between the spin measurements along axes \hat{a} or \hat{b} is

$$C(\hat{a}, \hat{b}) \coloneqq \left(\frac{2}{\hbar}\right)^2 \langle \psi | \, \hat{a} \cdot \hat{S}_{(1)} \otimes \hat{b} \cdot \hat{S}_{(2)} | \psi \rangle \tag{16.111}$$

where $\hat{S}_{(1)}$ and $\hat{S}_{(2)}$ are the spin operators for particles 1 and 2 respectively, and the tensor product is as we defined earlier in this chapter. Since the total angular momentum of the entangled vector $|\psi\rangle$ is zero, it is invariant under the unitary operators which generate rotations of the coordinate systems.

This means that $C(\hat{a}, \hat{b})$ is a function of $\hat{a} \cdot \hat{b} = \cos \theta_{ab}$ only and, hence, there is no loss of generality in assuming that \hat{a} points along the z-axis and that \hat{b} lies in the x - z plane. Then the expression for $C(\hat{a}, \hat{b})$ becomes

$$C(\hat{a}, b) = \langle \psi | \sigma_{1z} \otimes (\sigma_{2z} \cos \theta_{ab} + \sigma_{2x} \sin \theta_{ab}) | \psi \rangle$$
(16.112)

It is then straightforward to show that

$$C(\hat{a},\hat{b}) = -\cos\theta_{ab} \tag{16.113}$$

Now we restrict our attention to the special case in which (1) the four vectors $\hat{a}, \hat{a}', \hat{b}, \hat{b}'$ are coplanar and (2) \hat{a} or \hat{b} are parallel and (3) $\theta_{ab'} = \theta_{a'b} = \varphi$ say. Then the Bell inequality will be satisfied provided that

$$\left|1 + 2\cos\varphi - \cos 2\varphi\right| \le 2 \tag{16.114}$$

This is violated for all values of φ between 0° and 90°. This means that if the predictions of quantum theory are experimentally valid in this region then any idea of systems possessing individual values for observables must necessarily involve an essential non-locality. This applies in particular to any hidden variable theory that is completely consistent with the results of quantum theory. Thus, the important questions are:

- 1. Are the Bell inequalities empirically violated?
- 2. If so, are such violations in accord with the predictions of quantum theory?

In many experiments over the last two decades, the overwhelming conclusion is that the predictions of quantum theory *are* vindicated and so we are obliged either to stick with a pragmatic approach or a strict instrumentalist interpretation or else to accept the existence of a strange non-locality that seems hard to reconcile with our normal concepts of spatial separation between independent entities.

16.9 Bayesian Probability in QM

We turn to Bayesian probability arguments to deal with a realist.

16.9.1 Using Bayesian Ideas in Analysis of Experiments

In actual experimental tests, there are no infinite ensembles for accurate measurements of mean values. Experimental physicists perform a finite number of tests and then they state their results accompanied by a confidence level.

The real problem of theory versus experimental analysis is of a different nature however.

I am a theorist and I believe that quantum mechanics gives a reliable description of nature. I have a friend, however, who is a local realist.

We only have a finite number of trials of a Bell inequality experiment at our disposal.

How many tests are needed to make my realist friend feel uncomfortable?

The problem is not whether the validity of a Bell inequality can be salvaged by invoking clever loopholes, as some realists try to trick us into, but whether there can be any local realistic theory that reproduces the experimental results.

To simplify the discussion, I will assume that there are ideal detectors and that the rate at which particles are produced by the apparatus is perfectly known.

Experimental Results Change Beliefs

First, we consider a yes-no test.

Quantum mechanics(QM) predicts that the probability of the **yes** result is q and an alternative local realistic(LR) theory predicts a probability r.

An experimental test is performed n times and yields m yes results.

What can we infer about the likelihood of the two theories?

The answer is given by Baye's theorem

$$P(B|A \wedge C) = P(A|B \wedge C) \frac{P(B|C)}{P(A|C)}$$
(16.115)

Denote by $p'_q = P(q|I)$ and $p'_r = P(r|I)$ the prior probabilities that we assign to the validity of the two theories. These are subjective probabilities expressing our personal beliefs.

For example, if my friend is willing to bet 100 to 1 (for example) that LR is correct and QM is wrong, then

$$\frac{p'_r}{p'_q} = 100 \tag{16.116}$$

The question is: how many experimental tests are needed to change my friend's opinion to

$$\frac{p_r''}{p_q''} = 0.01 \tag{16.117}$$

say, before he is driven to bank ruptcy. This is a reversal (in belief) by a factor of $10^4.\,$

In this case, $P(r|\{m,n\} \land I) = p_r''$ is the new *prior* probability for my friend after the experiments are finished and similarly we have $P(q|\{m,n\} \land I) = p_q''$.

If we define

$$E_r = P(\{m, n\} | q \land I) \quad , \quad E_q = P(\{m, n\} | q \land I)$$
(16.118)

which are just the probabilities of the experimentally found result (the actual data - m successes in n trials) according to the two theories.

These follow from the binomial theorem

$$E_r = \frac{n!}{m!(n-m)!} r^m (1-r)^{n-m} , \quad E_q = \frac{n!}{m!(n-m)!} q^m (1-q)^{n-m}$$
(16.119)

It then follows from Baye's theorem that

$$P(\{m,n\}|r \wedge I)P(r|I) = P(r|\{m,n\} \wedge I)P(\{m,n\}|I)$$
(16.120)

$$P(\{m,n\}|q \wedge I)P(q|I) = P(q|\{m,n\} \wedge I)P(\{m,n\}|I)$$
(16.121)

or that

$$\frac{P(\{m,n\}|r \wedge I)P(r|I)}{P(r|\{m,n\} \wedge I)} = P(\{m,n\}|I) = \frac{P(\{m,n\}|q \wedge I)P(q|I)}{P(q|\{m,n\} \wedge I)}$$

or

$$\frac{P(\{m,n\}|r\wedge I)P(r|I)}{P(\{m,n\}|q\wedge I)P(q|I)} = \frac{p'_r E_r}{p'_q E_q} = \frac{P(r|\{m,n\}\wedge I)}{P(q|\{m,n\}\wedge I)} = \frac{p''_r}{p''_q}$$
(16.122)

We define the ratio

$$\frac{P(\{m,n\}|q \wedge I)}{P(\{m,n\}|r \wedge I)} = \frac{E_q}{E_r} = D = \left(\frac{q}{r}\right)^m \left(\frac{1-q}{1-r}\right)^{n-m}$$
(16.123)

as the *confidence depressing factor* for the hypothesis LR with respect to the hypothesis QM.

16.9.2 Simple Example

Suppose that we flip coins and the yes-no question is: Did the coin come up *heads*?

I, the theorist, will assume that the coin is unbiased and that therefore q = 0.5 and m = n/2 (assuming that I am correct). We then have

$$D = \left(\frac{1}{2r}\right)^{n/2} \left(\frac{1}{2(1-r)}\right)^{n/2} = \left(\frac{1}{2}\right)^n \left(\frac{1}{r(1-r)}\right)^{n/2}$$
(16.124)

Since we want 10^4 , we find

$$\left(\frac{5}{3}\right)^n = 10^4 \to n \log \frac{5}{3} = 4 \to n = \frac{4}{\log \frac{5}{3}} = \frac{4}{0.22} \approx 16$$
(16.125)

So that it would take only 16 coin flips to reverse my untrusting friend's belief.

Now let us return to the Bell inequality.



Figure 16.28: Three Detector Experiment

16.9.3 Simple Ideas

Let us consider a device that has three widely separated detectors each of which has two switch settings as shown in Figure 16.28 above.

When a detector is triggered it flashes either red or green. The detectors are far apart from the source, there are no connections between the detectors and no connections between the source and the detectors other than those mediated by the group of three particles (as shown) that originate at the source and fly away, one to each detector.

A run of the experiment consists of setting the switch on each detector to one of its two positions (labeled 1 or 2), pressing a button at the source (to release a trio of particles, one aimed at each detector), and recording the color subsequently flashed at each detector.

There are eight possible switch settings:

 $111 \ 112 \ 121 \ 122 \ 211 \ 212 \ 221 \ 222 \tag{16.126}$

We consider only the data acquired for four of the eight possible switch settings, namely, those in which the number of detectors set to 1 is odd.

$$111\ 122\ 212\ 221 \tag{16.127}$$

The other set

| $112 \ 1$ | 22 212 | 222 | (16.128) | |
|-----------|--------|-----|----------|--|
|-----------|--------|-----|----------|--|

will lead to similar results $(1 \leftrightarrow 2)$. As shown in Figure 16.28 we call the detectors A, B, and C, and specify pertinent facts about them by listing three pieces of information (switch settings or colors flashed) in that order.

If we run the experiment many times, then the observational results are the following. If just one detector is set to 1 (and the others to 2), then an odd number of red lights *always* flash, that is, either all three detectors flash red or there is one red flash and two green ones.

If all three detectors are set to 1, then an odd number of red lights is *never* observed to flash - either two of the three flash red or all three flash green.

| Settings | Result 1 | Result 2 | Result 3 | Result 4 |
|----------|----------|----------|----------|----------|
| 111 | GGG | GRR | RGR | RRG |
| 122 | RGG | GRG | GGR | RRR |
| 212 | RGG | GRG | GGR | RRR |
| 221 | RGG | GRG | GGR | RRR |

This is summarized by the table:

| Table 10.0. 10.50105 | Table | 16.3: | Results |
|----------------------|-------|-------|---------|
|----------------------|-------|-------|---------|

All four outcomes are *equally likely* in each case(this particular detail is not important).

We will discuss a real, physical system that exhibits this behavior later.

Let us set aside, for the moment, the 111 case and consider the 122, 212, and 221 cases in which just one detector is set to 1. Because an odd number of red lights always flash in any of these three cases, whenever the switches are so set we can predict with *certainty* what one of the three detectors will do in a run, merely by noting what happens to the other two. For should the other two flash the same color (RR or GG), then the third will have to flash red, but should the other two flash different colors (RG or GR), then the third will have to flash green.

Now we follow the path set out by EPR to draw an inference that will seem inescapable. Along the way we will use the so-called *EPR reality criterion*.

Since there are no direct connections between the detectors, their behavior can only be coordinated due to the fact that all three are triggered by particles that came from a common source. This fact and this fact alone must contain the explanation for why we can learn in advance what color will flash at a given detector, say A, from measurements made far away at B and C. Information telling the detector at A what color to flash in order to maintain the observed consistency with the colors flashed at B and C must somehow be *encoded* in the particle that triggers A. Since that particle could indeed have been coordinated with the particles that triggered B and C when all three were back at their common source, this explanation seems *both inevitable and entirely reasonable*.

We can apply this reasoning to any one of the three detectors (by moving it farther from the source so that before it flashes we have had the opportunity to observe what colors flash at the other two). We conclude that in each run of the experiment each particle *must* be carrying to its detector *instructions* on what color to flash, and that an odd number of the particles must specify red.

Thus, for a given choice of the switch settings (say 122) the particles heading for detectors A, B, and C must respectively be carrying instructions RRR, RGG, GRG, or GGR, but never GRR, RGR, RRG, or GGG.

Which of the four allowed groups of instructions they collectively carry is revealed only when the lights flash. All of the above reasoning applies equally well, of course, to 212 and 221 runs.

In the absence of connections between the detectors and the source, a particle has no information about how the switch of its detector will be set until it arrives there. Since in each run any detector might turn out to be the one set to 1 or one of the ones set to 2, to preserve the perfect record of always having an odd number of red flashes in 122, 212, and 221 runs, it would *seem to be essential* for each particle to be carrying instructions for how its detector should flash for *either* of the two possible switch settings it might find upon arrival.

The existence of *instructions* of this sort is the *EPR reality criterion*.

The instructions carried by each particle can be symbolized by a pair of letters

$$1 \to R \quad R \quad G \quad or \quad G$$
$$2 \to R \quad G \quad R \quad G$$

would result in RRR if the switch settings were 122, GGR for 212, and GRG for 221.

Since each of the three possible switch settings result in an odd number of red flashes, this is indeed a legal set of instructions.

An example of an illegal set of instructions is

$$\begin{array}{ccc} R & R & G \\ G & R & R \end{array}$$

for this gives an even number of red flashes GRR for the switch setting 212, which is never observed.

Since there are eight ways the lights can flash, namely,

RRR RRG RGG RGR GRR GRG GGG (16.129)

the total number of possible instruction sets is $8 \times 8 = 64$.

It is not hard to enumerate all the legal (odd number of red flashes) instruction sets.

First note that three of the six positions in a legal instruction set corresponding to any one of the three choices 122, 212, or 221 for the switch settings, must contain an odd number of R's, since that particular setting might be encountered in any run, and since only odd numbers of red flashes are ever observed. Thus, the only possible entries for the positions corresponding to the switch settings 122 are (leaving blank the entries not relevant to those three settings):

so that 122 gives RRR, RGG, GRG, or GGR independent of the other entries.

We can next count the way to fill in the blanks in these four forms so as to produce the correct data for switch settings 221. Since each of the four already specifies the color flashed at detector B for setting 2, namely, R G R G, to ensure that any 221 run produces an odd number of red flashes there are only two choices available for the other two (A and C) unspecified 221 entries for each of the four forms: RR or GG if the specified entry is R and RG or GR if the specified entry is G so that we have

This raises the number of possible forms to eight, each of which leaves only the entry for setting 1 at the detector B unspecified. But that entry is now entirely determined by the entries at settings 2 for detectors A and C (having to be R,

if the latter two entries are the same color and G, if they are different).

| | ABC | ABC | ABC | ABC |
|-----------------|-----|-----|----------------------|----------------------|
| $1 \rightarrow$ | RRR | RGG | GRG | GGR |
| $2 \rightarrow$ | RRR | RGG | GRG | GGR |
| | ABC | ABC | ABC | ABC |
| $1 \rightarrow$ | RGR | RRR | GGR | GRG |
| $2 \rightarrow$ | RRR | GGG | RRG | RGR |

They are arranged in the same horizontal order as the forms in (1), with the two possibilities for each form placed directly above one another. It is easy to check explicitly that each instruction set (2) does indeed give an odd number of red flashes when a single detector is set to 1.

| 122 | gives | RRR | RGG | GRG | GGR |
|-----|-------|-----|-----|-----|----------------------|
| | | RRR | RGG | GRG | GGR |
| 221 | gives | RRR | RGG | GRG | GGR |
| | | GRG | GGR | RRR | RGG |
| 212 | gives | RRR | RGG | GRG | GGR |
| | | GGR | GRG | RGG | RRR |

Clearly, (2) represents the eight legal sets.

Now, finally, we consider the fourth type of run, in which all three detectors are set to 1, and an odd number of red flashes is never observed.

The above instruction sets must determine the outcomes of these runs as well. For who is to prevent somebody from flipping the two switches set to 2 over to 1, just before the particles arrive?

An inspection of the upper rows in (2) reveals that every one of the eight allowed instruction sets results in an odd number of red flashes when all three switches are set to 1.

If the instruction sets existed, then 111 runs would *always* have to produce an odd number of red flashes. But they *never* do.

Thus, a *single* 111 run suffices all by itself to give data inconsistent with the otherwise compelling inference of instruction sets.

Here the instruction sets(realistic theory) *require* an odd number of red flashes in *every* 111 run, but quantum mechanics(experiment) *prohibits* an odd number of red flashes in *every* 111 run. Something is wrong with the EPR idea of *instruction* sets or EPR reality.

The Quantum Mechanical Explanation

Here is how the device works. What emerges from the source are three spin-1/2 particles (a, b, and c) in a spin state whose structure is given below. The particles fly apart to the detectors in the horizontal plane. We define the z-direction for each particle to be along the line of flight. The detectors contain Stern-Gerlach magnets which measure the vertical (x) component of the spin when the switch is set to 1 and the horizontal component (y) perpendicular to the line of flight when their switch is set to 2. They are set so that we get red flashes for spin-up, and green flashes for spin-down.

Let us describe a spin state that produces the remarkable correlations (GHZ-state) described earlier.

We measure angular momentum for each particle in units of ? so that the spin operators for each particle can be taken to be the Pauli matrices. Now consider the three commuting Hermitian operators

$$\sigma_x^a \sigma_y^b \sigma_y^c \quad , \quad \sigma_y^a \sigma_x^b \sigma_y^c \quad , \quad \sigma_y^a \sigma_y^b \sigma_x^c \tag{16.130}$$

They commute because all pairs of the six spin operators out of which they are constructed commute, except for those associated with the x and y components of the spin of a single particle, which anticommute. This does not cause any trouble, however, because converting the product in one order to the product in then other order always involves and even number of such anticommuting exchanges.

Being commuting and Hermitian, the three operators above can be provided with simultaneous eigenvectors. Since the square of each operator is the identity, the eigenvalues of each can only be ± 1 .

The actual spin state that produces the remarkable correlations (the *Greenberger-Horne-Zeilinger or GHZ-state*) is described by

$$|GHZ\rangle = \frac{1}{\sqrt{2}} (|1,1,1\rangle - |-1,-1,-1\rangle)$$
 (16.131)

where ± 1 specifies spin-up or spin-down along the appropriate z-axis.

For simplicity in the following argument, here we pick the state with all three eigenvalues equal to +1, which preserves the symmetry among the particles. The argument works for any such symmetric state and for any linear combination of such states as in the above state.

Since the components of the spin vectors of different particles commute, we can

simultaneously measure the x component for one particle and the y components for the other two. Because the spin state is an eigenvector of all three of the operators

$$\sigma^a_x \sigma^b_y \sigma^c_y$$
 , $\sigma^a_y \sigma^b_x \sigma^c_y$, $\sigma^a_y \sigma^b_y \sigma^c_x$

with eigenvalue +1, the product of the results of each of the three single spin measurements has to be +1, regardless of which particle we pick for the x spin measurement. Since +1 flashes red and -1 flashes green, there must indeed be an even number of green flashes and thus an odd number of red flashes.

What about the result of three x-spin measurements, declared earlier never to result in an odd number of red flashes? Translating this into spin language tells us that the product of the three results must always be -1. The Hermitian operator corresponding to that product is

$$\sigma_x^a \sigma_x^b \sigma_x^c \tag{16.132}$$

so for the declaration to be correct, it must be that the eigenvector of the first three operators with eigenvalue +1 is also an eigenvector of the last operator(above) with eigenvalue -1.

This is easily confirmed. Indeed, the last operator is just minus the product of the other three operators

$$\sigma_x^a \sigma_x^b \sigma_x^c = -(\sigma_x^a \sigma_y^b \sigma_y^c)(\sigma_y^a \sigma_x^b \sigma_y^c)(\sigma_y^a \sigma_y^b \sigma_x^c)$$
(16.133)

Since we are in an eigenvector with eigenvalue +1 of each of the three operators appearing on the right, we are indeed also in an eigenvector of $\sigma_x^a \sigma_x^b \sigma_x^c$ with eigenvalue -1.

The consequence of the EPR reality criterion specified earlier, if translated into quantum theoretic terminology, would also assert that the state was an eigenvector of the operator $\sigma_x^a \sigma_x^b \sigma_x^c$, but with the wrong eigenvalue. In this sense, the GHZ experiment provides the strongest possible contradiction between quantum mechanics and the EPR reality criterion.

Alternatively, we can say it this way. We may measure, on each particle, either σ_x or σ_y , without disturbing the other particles. The results of these measurements will be called m_x or m_y , respectively. From

$$\sigma_x^a \sigma_y^b \sigma_y^c |111\rangle = |111\rangle$$

$$\sigma_y^a \sigma_x^b \sigma_y^c |111\rangle = |111\rangle$$

$$\sigma_y^a \sigma_y^b \sigma_x^c |111\rangle = |111\rangle$$

$$\sigma_x^a \sigma_x^b \sigma_x^c |111\rangle = -|111\rangle$$

and

we can predict with certainty that, if the three σ_x are measured, the results satisfy

$$m_{ax}m_{bx}m_{cx} = -1$$
 (16.134)

Therefore, each of the operators σ_x^a , σ_x^b and σ_x^c corresponds to an EPR element of reality, because its value can be predicted with certainty by performing measurements on the two *other*, distant particles.

However, it follows from

$$\begin{aligned} \sigma_x^a \sigma_y^b \sigma_y^c &|111\rangle = |111\rangle \\ \sigma_y^a \sigma_x^b \sigma_y^c &|111\rangle = |111\rangle \\ \sigma_y^a \sigma_y^b \sigma_x^c &|111\rangle = |111\rangle \end{aligned}$$

that we can predict with certainty the value of σ_x^a by measuring σ_y^b and σ_y^c rather than σ_x^b and σ_x^b . We then have

$$m_{ax}m_{by}m_{cy} = +1$$
 (16.135)

and likewise, by cyclic permutation,

$$m_{ay}m_{bx}m_{cy} = +1$$
 (16.136)

and

$$m_{ay}m_{by}m_{cx} = +1$$
 (16.137)

The product of the last four results gives

$$m_{ax}m_{bx}m_{cx}m_{ax}m_{by}m_{cy}m_{ay}m_{bx}m_{cy}m_{ay}m_{by}m_{cx} = -1$$
(16.138)

$$(m_{ax})^2 (m_{bx})^2 (m_{cx})^2 (m_{by})^2 (m_{cy})^2 (m_{ay})^2 = -1$$
(16.139)

But,

$$(m_{jx})^2 = 1 \tag{16.140}$$

so that we get a contradiction.

There is a tacit assumption in the above argument, that $m_{ax} \ln m_{ax} m_{bx} m_{cx} = -1$ is the same as $m_{ax} \ln m_{ax} m_{by} m_{cy} = +1$, in spite of the fact that these two ways of obtaining m_{ax} involve mutually exclusive experiments - measuring σ_x^b and σ_x^c or measuring σ_y^b and σ_y^c .

This tacit assumption is of counterfactual nature, and cannot be experimentally verified. It obviously adheres to the EPR reality criterion - but is simply wrong!

Saying it another way, the crucial minus sign in

$$\sigma_x^a \sigma_x^b \sigma_x^c = -(\sigma_x^a \sigma_y^b \sigma_y^c) (\sigma_y^a \sigma_x^b \sigma_y^c) (\sigma_y^a \sigma_y^b \sigma_x^c)$$

which is totally destructive of the possibility of these instruction sets, comes from the fact that in working out the identity it is necessary to interchange the anticommuting operators σ_x^b and σ_y^b in order to get rid of all the *y* components (using $(\sigma_y^i)^2 = 1$) and be left with a product of three *x* components. It is only that one instance of uncompensated anticommutation that produces the conclusion so devastating to the hypothesis of instruction sets.

This is extremely pleasing, for it is just the fact the x and y components of the spin of a single particle do not commute, which leads the well-educated quantum mechanician to reject from the start the inference instruction sets (which have to specify the value of both of these non-commuting observables), making it necessary for me to disguise what was going on earlier so that you would not have dismissed this discussion as rubbish before reaching the interesting part.

There is no other Bellian refutation of EPR in which the mathematical details of the refutation so closely reflect the broad interpretive doctrines of quantum theory that EPR tried to challenge. The entries in the instruction sets are precisely the conjectured *c*-number values for all the σ_x^i and σ_y^i -values that appear to be the only explanation for the remarkable correlations. In addition, the logic of the red and green lights in the simple model precisely parallels the algebraic behavior of the four operators used here except for that one devastating anticommutation.

Let us return now to using Bayesian ideas to convince our realist friends about the validity of quantum mechanics within the context of the Bell inequalities.

16.9.4 More about the Greenberger-Horne-Zeilinger(GHZ) State

We consider the GHZ state for a three-particle system

$$|GHZ\rangle = \frac{1}{\sqrt{2}}(|1,1,1\rangle - |-1,-1,-1\rangle)$$
 (16.141)

where -1 and +1 denote any two orthogonal states of each of the three particle subsystems.

We have three distant observers examine the three subsystems. The first observer has the choice of two tests. The first test can give two different results that we label $a = \pm 1$, and likewise the other test yields $a' = \pm 1$. Symbols b, b', c and c' are similarly defined for the other two observers. Any possible values of their results satisfy

$$a'bc = ab'c = abc' = -a'b'c' = +1$$
(16.142)

Mermin has then shown that we have the inequality

$$-2 \le \langle a'bc + ab'c + abc' - a'b'c' \rangle \le +2 \tag{16.143}$$

As we saw above quantum mechanics makes a very simple prediction for the GHZ state: there are well chosen tests that give with certainty

$$a'bc = ab'c = abc' = -a'b'c' = +1$$
(16.144)

It is important to remember that performing any such test can verify the value 1 for only one of these products (at a time) since each product corresponds to a different experimental setup.

If, however, we take all these results together, they manifestly conflict with $a'bc + ab'c + abc' - a'b'c' = \pm 2$.

Many physicists have erroneously, at this point, stated that a single experiment is sufficient to invalidate local realism. This is sheer nonsense: a single experiment can only verify one occurrence of one of the terms in

$$a'bc = ab'c = abc' = -a'b'c' = +1 \tag{16.145}$$

What does our realist friend think?

He believes that, in each experimental run, each term in the above result has a definite value even if that term is not actually measured in that run.

We ask him to propose a rule giving the *average* values of the products in

$$a'bc + ab'c + abc' - a'b'c' = \pm 2 \tag{16.146}$$

Suppose that he assumes

$$\langle a'bc \rangle = \langle ab'c \rangle = \langle abc' \rangle = \langle -a'b'c' \rangle = 0.5 \tag{16.147}$$

This clearly attains the right hand side of (Mermin's) inequality. This assumption then leads to the prediction that if we measure a'bc we shall find the result 1 (that is, *yes*) in 75% of the cases and the opposite result in 25% and like wise for the other tests. This simply corresponds to the averages proposed above.

In our earlier discussion about confidence depressing factors, this corresponds to

$$q = 1 \text{ and } r = 0.75$$
 (16.148)

If we assume that quantum mechanics is correct, then m = n (that is what q = 1 means). Therefore, we have

$$D = \left(\frac{q}{r}\right)^m \left(\frac{1-q}{1-r}\right)^{n-m} = \left(\frac{1}{r}\right)^n = \left(\frac{4}{3}\right)^n \tag{16.149}$$

Therefore it would take

$$D = \left(\frac{4}{3}\right)^n = 10^4 \to n = \frac{4}{\log(1.33)} \approx 32 \tag{16.150}$$

tests to undo the realist's beliefs.

16.10 Problems

16.10.1 Bell Inequality with Stern-Gerlach

A pair of spin-1/2 particles is produced by a source. The spin state of each particle can be measured using a Stern-Gerlach apparatus (see diagram below).



Figure 16.29: EPR Stern-Gerlach Setup

(a) Let \hat{n}_1 and \hat{n}_2 be the field directions(arrows in diagram) of the Stern-Gerlach magnets. Consider the commuting observables

$$\sigma^{(1)} = \frac{2}{\hbar} \hat{n}_1 \cdot \vec{S}_1 \quad , \quad \sigma^{(2)} = \frac{2}{\hbar} \hat{n}_2 \cdot \vec{S}_2$$

corresponding to the spin component of each particle along the direction of the Stern-Gerlach apparatus associated with it. What are the possible values resulting from measurement of these observables and what are the corresponding eigenstates?

(b) Consider the observable $\sigma^{(12)} = \sigma^{(1)} \otimes \sigma^{(2)}$ and write down its eigenvectors and eigenvalues. Assume that the pair of particles is produced in the singlet state

$$|0,0\rangle = \frac{1}{\sqrt{2}} \left(|S_z+\rangle^{(1)} |S_z-\rangle^{(2)} - |S_z-\rangle^{(1)} |S_z+\rangle^{(2)} \right)$$

What is the expectation value of $\sigma^{(12)}$?

(c) Make the assumption that the spin of a particle has a meaningful value even when it is not being measured. Assume also that the only possible results of the measurement of a spin component are $\pm \hbar/2$. Then show that the probability of finding the spins pointing in two given directions will be proportional to the overlap of the hemispheres that these two directions define. Quantify this criterion and calculate the expectation value of $\sigma^{(12)}$.

(d) Assume the spin variables depend on a *hidden variable* λ . The expectation value of the spin observable $\sigma^{(12)}$ is determined in terms of the normalized distribution function $f(\lambda)$:

$$\left\langle \sigma^{(12)} \right\rangle = \frac{4}{\hbar^2} \int d\lambda f(\lambda) S_z^{(1)}(\lambda) S_{\varphi}^{(2)}(\lambda)$$

Prove Bell's inequality

$$\left|\left\langle\sigma^{(12)}(\varphi)\right\rangle - \left\langle\sigma^{(12)}(\varphi')\right\rangle\right| \le 1 + \left|\left\langle\sigma^{(12)}(\varphi - \varphi')\right\rangle\right|$$

(e) Consider Bell's inequality for $\varphi' = 2\varphi$ and show that it is not true when applied in the context of quantum mechanics.

16.10.2 Bell's Theorem with Photons

Two photons fly apart from one another, and are in oppositely oriented circularly polarized states. One strikes a polaroid film with axis parallel to the unit vector \hat{a} , the other a polaroid with axis parallel to the unit vector \hat{b} . Let $P_{++}(\hat{a},\hat{b})$ be the joint probability that both photons are transmitted through their respective polaroids. Similarly, $P_{--}(\hat{a},\hat{b})$ is the probability that both photons are absorbed by their respective polaroids, $P_{+-}(\hat{a},\hat{b})$ is the probability that the photon at the \hat{a} polaroid is transmitted and the other is absorbed, and finally, $P_{-+}(\hat{a},\hat{b})$ is the probability that the photon at the \hat{a} polaroid is absorbed and the other is transmitted.

The classical realist assumption is that these probabilities can be separated:

$$P_{ij}(\hat{a},\hat{b}) = \int d\lambda \rho(\lambda) P_i(\hat{a},\lambda) P_j(\hat{b},\lambda)$$

where *i* and *j* take on the values + and –, where λ signifies the so-called hidden variables, and where $\rho(\lambda)$ is a weight function. This equation is called the separable form.

The correlation coefficient is defined by

$$C(\hat{a},\hat{b}) = P_{++}(\hat{a},\hat{b}) + P_{--}(\hat{a},\hat{b}) - P_{+-}(\hat{a},\hat{b}) - P_{-+}(\hat{a},\hat{b})$$

and so we can write

$$C(\hat{a},\hat{b}) = \int d\lambda \rho(\lambda) C(\hat{a},\lambda) C(\hat{b},\lambda)$$

where

$$C(\hat{a},\lambda) = P_+(\hat{a},\lambda) - P_-(\hat{a},\lambda) \quad , \quad C(\hat{b},\lambda) = P_+(\hat{b},\lambda) - P_-(\hat{b},\lambda)$$

It is required that
- (a) $\rho(\lambda) \ge 0$
- (b) $\int d\lambda \rho(\lambda) = 1$
- (c) $-1 \le C(\hat{a}, \lambda) \le 1$, $-1 \le C(\hat{b}, \lambda) \le 1$

The Bell coefficient

$$B = C(\hat{a}, \hat{b}) + C(\hat{a}, \hat{b}') + C(\hat{a}', \hat{b}) - C(\hat{a}', \hat{b}')$$

combines four different combinations of the polaroid directions.

- (1) Show that the above classical realist assumptions imply that $|B| \leq 2$
- (2) Show that quantum mechanics predicts that $C(\hat{a}, \hat{b}) = 2(\hat{a} \cdot \hat{b})^2 1$
- (3) Show that the maximum value of the Bell coefficient is $2\sqrt{2}$ according to quantum mechanics
- (4) Cast the quantum mechanical expression for $C(\hat{a}, \hat{b})$ into a separable form. Which of the classical requirements, (a), (b), or (c) above is violated?

16.10.3 Bell's Theorem with Neutrons

Suppose that two neutrons are created in a singlet state. They fly apart; the spin of one particle is measured in the direction a, the other in the direction b.

- (a) Calculate the relative frequencies of the coincidences R(up, up), R(up, down), R(down, up) and R(down, down), as a function of θ , the angle between a and b.
- (b) Calculate the correlation coefficient

C(a,b) = R(up, up) - R(up, down) - R(down, up) + R(down, down)

(c) Given two possible directions, a and a', for one measurement, and two possible directions, b and b', for the other, deduce the maximum possible value of the Bell coefficient, defined by

$$B = C(a,b) + C(a',b) + C(a',b') - C(a,b')$$

(d) Show that this prediction of quantum mechanics is inconsistent with classical local realism.

16.10.4 Greenberger-Horne-Zeilinger State

The Greenberger-Horne-Zeilinger (GHZ) state of three identical spin-1/2 particles is defined by

$$|GHZ\rangle = \frac{1}{\sqrt{2}} \left(|z_a + \rangle |z_b + \rangle |z_c + \rangle - |z_a - \rangle |z_b - \rangle |z_c - \rangle \right)$$

where z_a + is the eigenvector of the z-component of the spin operator of particle a belonging to eigenvalue $+\hbar/2$ (z-spin up), z_a - is the eigenvector of the z-component of the spin operator of particle a belonging to eigenvalue $-\hbar/2$ (z-spin down), and similarly for b and c. Show that, if spin measurements are made on the three particle in the x- or y-directions,

- (a) the product of three spins in the x-direction is always $-\hbar^3/8$
- (b) the product of two spins in the y-direction and one spin in the x-direction is always $+\hbar^3/8$
- (c) Consider a prize game for a team of three players, A, B, and C. The players are told that they will be separated from one another and that each will be asked one of two questions, say X or Y, to which each must give one of two allowed answers, namely, +1 or −1. Moreover, *either*
 - (a) all players will be asked the same question X

or

(b) one of the three players will be asked X and the other two Y

After having been asked X or Y, no player may communicate with the others until after all three players have given their answers, +1 or -1. To win the game, the players must give answers such that, in case (a) the product of the three answers is -1, whereas in case (b) the product of the three answers is +1.

- (a) Show that no classical strategy gives certainty of a win for the team
- (b) Show that a quantum strategy, in which each player may take one of the GHZ particles with her, exists for which a win is certain

Chapter 17

Path Integral Methods

17.1 Historical Remarks

In this book we have developed the standard formulation of quantum mechanics developed more or less concurrently by Schrodinger, Heisenberg, Dirac and others in the 1920s and shown to be equivalent to one another soon thereafter.

In 1933, Dirac made the observation that the action plays a central role in classical mechanics (he considered the Lagrangian formulation of classical mechanics to be more fundamental than the Hamiltonian formulation), but that it seemed to have no important role in quantum mechanics as it was known at the time. He speculated on how the situation might be rectified, and he arrived at the conclusion that (in more modern language) the propagator in quantum mechanics *corresponds to*

$$\exp\left(i\frac{S}{\hbar}\right) \tag{17.1}$$

where S is the classical action evaluated along the classical path.

In 1948, Feynman developed Dirac's suggestion, and succeeded in deriving a new formulation of quantum mechanics, based on the fact that the propagator can be written as a sum over all possible paths (not just the classical one) between the initial and final points. Each path contributes $\exp(iS/\hbar)$ to the propagator. So while Dirac considered only the classical path, Feynman showed that all paths contribute: in a sense, the quantum particle takes all paths, and the amplitudes for each path add according to the usual quantum mechanical rule for combining amplitudes.

17.2 Motivation

What do we learn from path integrals? Path integrals give us no dramatic new results in the quantum mechanics of a single particle. In fact, most, if not all,

calculations in quantum mechanics which can be done by path integrals can be done with considerably greater ease using the standard formulation of quantum mechanics. So why all the fuss?

It turns out that path integrals are considerably more useful in more complicated situations, such as quantum field theory. Even if this was not case, however, path integrals give a very worthwhile contribution to our understanding of quantum mechanics.

First, path integrals provide a physically extremely appealing and intuitive way of viewing quantum mechanics: anyone who can understand Young's double slit experiment in optics should be able to understand the underlying ideas behind path integrals.

Second, the classical limit of quantum mechanics can be understood in a particularly clean way via path integrals.

17.3 Path Integrals in Quantum Mechanics

17.3.1 General ideas

Consider a particle moving in one dimension. The Hamiltonian has the usual form:

$$H = \frac{p^2}{2m} + V(q)$$
 (17.2)

The fundamental question in the path integral (PI) formulation of quantum mechanics is:

If the particle is at a position q at time t = 0, what is the probability amplitude that it will be at some other position q' at a later time t = T?

It is easy to get a formal expression for this amplitude in the usual Schrödinger formulation of quantum mechanics. Let us introduce the eigenstates of the position operator \hat{q} , which form a complete orthonormal set:

$$\hat{q}|q\rangle = q|q\rangle$$
 , $\langle q'|q\rangle = \delta(q'-q)$, $\int dq|q\rangle\langle q| = 1$ (17.3)

(when there is the possibility of an ambiguity, operators will be written with a *hat*, otherwise the hat will be dropped). Then the initial state is

$$|\psi(0)\rangle = |q\rangle \tag{17.4}$$

Letting the state evolve in time and projecting on the state $|q'\rangle$, we get the amplitude A,

$$A = \langle q' | \psi(T) \rangle \equiv K(q', T; q, 0) = \langle q' | e^{-iHT} | q \rangle$$
(17.5)

(except where otherwise noted, \hbar will be set to 1). This object, for obvious reasons, is known as the propagator from the initial space-time point (q, 0) to the final point (q', T). Clearly, the propagator is independent of the origin of time:

$$K(q', T+t; q, t) = K(q', T; q, 0)$$
(17.6)

We will derive an expression for this amplitude in the form of a summation (integral really) over all possible paths between the initial and final points. In doing so, we will derive the PI method from quantum mechanics.

Let us separate the time evolution in the above amplitude into two smaller time evolutions, writing

$$e^{-iHT} = e^{-iH(T-t_1)}e^{-iHt_1} \tag{17.7}$$

The amplitude becomes

$$A = \langle q' | e^{-iH(T-t_1)} e^{-iHt_1} | q \rangle$$
(17.8)

Inserting an identity operator gives

$$A = \int dq_1 \langle q' | e^{-iH(T-t_1)} | q_1 \rangle \langle q_1 | e^{-iHt_1} | q \rangle$$

= $\int dq_1 K(q', T; q_1, t_1) K(q_1, t_1; q, 0)$ (17.9)

This formula is none other than an expression of the quantum mechanical rule for combining amplitudes. If a process can occur a number of ways, the amplitude for each of these ways add. A particle, in propagating from q to q', must be somewhere at an intermediate time t_1 . Labelling that intermediate position q_1 , we compute the amplitude for propagation via the point q_1 (this is the product of two propagators as in equation(17.9)) and integrate over all possible intermediate positions. This result is reminiscent of Young's double slit experiment where the amplitudes for passing through each of the two slits combine and interfere. We will look at this example in more detail later.

We can repeat the division of the time interval T. Let us divide it up into a large number N of time intervals of duration $\delta = T/N$. Then we can write the propagator as

$$A = \langle q' | \left(e^{-iH\delta} \right)^N | q \rangle = \langle q' | \underbrace{e^{-iH\delta} e^{-iH\delta} \dots e^{-iH\delta}}_{\text{Ntimes}} | q \rangle$$
(17.10)

We can again insert a complete set of states (identity operator) between each exponential, which gives

$$\begin{aligned} A &= \langle q' | e^{-iH\delta} \int dq_{N-1} | q_{N-1} \rangle \langle q_{N-1} | e^{-iH\delta} \int dq_{N-2} | q_{N-2} \rangle \langle q_{N-2} | \dots \dots \dots \\ & \dots \int dq_2 | q_2 \rangle \langle q_2 | e^{-iH\delta} \int dq_1 | q_1 \rangle \langle q_1 | e^{-iH\delta} | q \rangle \\ &= \int dq_1 \dots \dots dq_{N-1} \langle q' | e^{-iH\delta} | q_{N-1} \rangle \langle q_{N-1} | e^{-iH\delta} | q_{N-2} \rangle \dots \dots \langle q_1 | e^{-iH\delta} | q \rangle \\ &= \int dq_1 \dots \dots dq_{N-1} K_{q_N, q_{N-1}} K_{q_{N-1}, q_{N-2}} \dots \dots K_{q_2, q_1} K_{q_1, q_0} \end{aligned}$$

where we have defined $q_0 = q$, $q_N = q'$ and $K_{q_i, q_j} = \langle q_j | e^{-iH\delta} | q_i \rangle$. Note that the initial and final positions are not integrated over. This expression says that the amplitude is the integral of the amplitude of all *N*-legged paths, as illustrated in Figure 17.1 below



Figure 17.1: Amplitude as a sum over N-legged paths

Apart from the mathematical details concerning the limit $N \to \infty$, this is clearly going to become a sum over all possible paths of the amplitude for each path:

$$A = \sum_{paths} A_{path} \tag{17.11}$$

where

$$\sum_{paths} = \int dq_1 \dots dq_{N-1} \quad , \quad A_{path} = K_{q_N, q_{N-1}} K_{q_{N-1}, q_{N-2}} \dots K_{q_2, q_1} K_{q_1, q_0}$$
(17.12)

Let us look at this expression in detail.

The propagator for one sub-interval is

$$K_{q_{j+1}, q_j} = \langle q_{j+1} | e^{-iH\delta} | q_j \rangle$$
(17.13)

We can expand the exponential, since ? is small:

$$K_{q_{j+1}, q_j} = \langle q_{j+1} | e^{-iH\delta} | q_j \rangle = \langle q_{j+1} | \left(1 - iH\delta - \frac{1}{2}H^2\delta^2 + \dots \right) | q_j \rangle$$

= $\langle q_{j+1} | q_j \rangle - i\delta \langle q_{j+1} | H | q_j \rangle + O(\delta^2)$ (17.14)

The first term is a delta function, which we can write as

$$\langle q_{j+1} | q_j \rangle = \delta (q_{j+1} - q_j) = \int \frac{dp_j}{2\pi} e^{ip_j(q_{j+1} - q_j)}$$
 (17.15)

In the second term of equation(17.14), we can insert another identity operator but this time in the form of an integral over momentum eigenstates between Hand $|q_j\rangle$. This gives

$$-i\delta \langle q_{j+1} | H | q_j \rangle = -i\delta \langle q_{j+1} | \left(\frac{p^2}{2m} + V(q) \right) \left(\int \frac{dp_j}{2\pi} | p_j \rangle \langle p_j | \right) | q_j \rangle$$
$$= -i\delta \int \frac{dp_j}{2\pi} \langle q_{j+1} | \left(\frac{p^2}{2m} + V(q) \right) | p_j \rangle \langle p_j | q_j \rangle$$
$$= -i\delta \int \frac{dp_j}{2\pi} \langle q_{j+1} | \left(\frac{p_j^2}{2m} + V(q_{j+1}) \right) | p_j \rangle \langle p_j | q_j \rangle$$
$$= -i\delta \int \frac{dp_j}{2\pi} \left(\frac{p_j^2}{2m} + V(q_{j+1}) \right) \langle q_{j+1} | p_j \rangle \langle p_j | q_j \rangle$$
$$= -i\delta \int \frac{dp_j}{2\pi} \left(\frac{p_j^2}{2m} + V(q_{j+1}) \right) e^{ip_j(q_{j+1}-q_j)}$$
(17.16)

where we used $\langle q | p \rangle = \exp(ipq)$. Note that the operator p acted to the right and the operator V(q) acted to the left.

The expression in equation (17.16) is asymmetric between q_{j+1} and q_j . The origin of this is our choice of putting the identity operator to the right of H in the second term of equation (17.14). Had we put it to the left instead, we would have obtained $V(q_j)$ in equation (17.16). To not play favorites, we should choose some sort of average of these two cases. In what follows, I will simply write $V(\bar{q}_j)$ where $\bar{q}_j = \frac{1}{2} (q_{j+1} + q_j)$ (the exact choice does not matter in the continuum limit, which we will take eventually; this choice is the common choice). Combining equations (17.15) and (17.16), the sub-interval propagator is

$$K_{q_{j+1}, q_j} = \int \frac{dp_j}{2\pi} e^{ip_j(q_{j+1}-q_j)} \left(1 - i\delta \left(\frac{p_j^2}{2m} + V(\bar{q}_j) \right) + O(\delta^2) \right)$$
$$= \int \frac{dp_j}{2\pi} e^{ip_j(q_{j+1}-q_j)} e^{-i\delta H(p_j, \bar{q}_j)} \left(1 + O(\delta^2) \right)$$
(17.17)

There are N such factors in the amplitude. Combining them, and writing $\dot{q}_j = (q_{j+1} - q_j)/\delta$, we get

$$A_{path} = \int \prod_{j=0}^{N-1} \frac{dp_j}{2\pi} \exp\left(i\delta \sum_{j=0}^{N-1} \left(p_j \dot{q}_j - H(p_j \,, \, \bar{q}_j)\right)\right)$$
(17.18)

where we have neglected a multiplicative factor of the form $(1 + O(\delta^2))^N$ which will tend toward one in the continuum limit. Then the propagator becomes

$$K = \int dq_1 \dots dq_{N-1} A_{path}$$

= $\int \prod_{j=1}^{N-1} dq_j \int \prod_{j=0}^{N-1} \frac{dp_j}{2\pi} \exp\left(i\delta \sum_{j=0}^{N-1} (p_j \dot{q}_j - H(p_j, \bar{q}_j))\right)$ (17.19)

Note that there is one momentum integral for each interval (N total), while there is one position integral for each intermediate position (N - 1 total).

If $N \to \infty$, this approximates an integral over all functions p(t), q(t). We adopt the following notation:

$$K \equiv \int Dp(t)Dq(t) \exp\left(i\int_{0}^{T} dt \left(p\dot{q} - H(p, q)\right)\right)$$
(17.20)

This result is known as the phase-space path integral. The integral is viewed as over all functions p(t) and over all functions q(t) where q(0) = q, q(T) = q'. But to actually perform an explicit calculation, equation(17.20) should be viewed as a shorthand notation for the expression equation(17.19) in the limit $N \to \infty$.

If, as is often the case (and we have assumed in deriving the above expression), the Hamiltonian is of the standard form, namely

$$H = \frac{p^2}{2m} + V(q)$$
 (17.21)

we can actually carry out the momentum integrals in equation (17.19). We can rewrite this expression as

$$K = \int \prod_{j=1}^{N-1} dq_j \exp\left(-i\delta \sum_{j=0}^{N-1} V(\bar{q}_j)\right) \int \prod_{j=0}^{N-1} \frac{dp_j}{2\pi} \exp\left(i\delta \sum_{j=0}^{N-1} \left(p_j \dot{q}_j - \frac{p_j^2}{2m}\right)\right)$$
(17.22)

The p integrals are all Gaussian, and they are uncoupled. One such integral is

$$\int \frac{dp}{2\pi} e^{i\delta(p\dot{q}-p^2/2m)} = \sqrt{\frac{m}{2\pi i\delta}} e^{i\delta m\dot{q}^2/2}$$
(17.23)

The careful reader may be worried about the convergence of this integral. If so, a factor $\exp(-\varepsilon p^2)$ can be introduce and the limit $\varepsilon \to 0$ taken at the end (see

for example Chapter 1 - page 21).

The propagator becomes

$$K = \int \prod_{j=1}^{N-1} dq_j \exp\left(-i\delta \sum_{j=0}^{N-1} V(\bar{q}_j)\right) \prod_{j=0}^{N-1} \left(\sqrt{\frac{m}{2\pi i\delta}} \exp\left(\frac{i\delta m \dot{q}_j^2}{2}\right)\right)$$
$$= \left(\frac{m}{2\pi i\delta}\right)^{N/2} \int \prod_{j=1}^{N-1} dq_j \exp\left(i\delta \sum_{j=0}^{N-1} \left(\frac{m \dot{q}_j^2}{2} - V(\bar{q}_j)\right)\right)$$
(17.24)

The argument of the exponential is a discrete approximation of the **action** of a path passing through the points $q_0 = q, q_1, ..., q_{N-1}, q_N = q'$. As above, we can write this in the more compact form

$$K = \int Dq(t) \exp\left(iS(q(t))\right) \tag{17.25}$$

This is our final result and is known as the configuration space path integral. Again, equation(17.25) should be viewed as a notation for the more precise expression equation(17.24), as $N \to \infty$.

17.3.2 Examples

To solidify the above notions, let us consider a few explicit examples. As a first example, we will compute the free particle propagator first using ordinary quantum mechanics and then via PI. We will then mention some generalization which can be done in a similar manner.

Free Particle

Let us compute the propagator K(q',T;q,0) for a free particle, described by the Hamiltonian

$$H = \frac{p^2}{2m} \tag{17.26}$$

The propagator can be computed straightforwardly using ordinary quantum mechanics. To this end, we write

$$K = \langle q' | e^{-iHT} | q \rangle = \langle q' | e^{-ip^2 T/2m} \int \frac{dp}{2\pi} | p \rangle \langle p | q \rangle$$
$$= \int \frac{dp}{2\pi} e^{-ip^2 T/2m} \langle q' | p \rangle \langle p | q \rangle = \int \frac{dp}{2\pi} e^{-ip^2 T/2m + i(q'-q)p}$$
(17.27)

The integral is a Gaussian. We obtain

$$K = \left(\frac{m}{2\pi i T}\right)^{1/2} e^{im(q'-q)^2/2T}$$
(17.28)

Let us see how the same result can be obtained using PIs. The configuration space PI (equation(17.25)) is

$$K = \lim_{N \to \infty} \left(\frac{m}{2\pi i \delta} \right)^{N/2} \int \prod_{j=1}^{N-1} dq_j \exp\left(i \frac{m \delta}{2} \sum_{j=0}^{N-1} \left(\frac{q_{j+1} - q_j}{\delta} \right)^2 \right)$$
$$= \lim_{N \to \infty} \left(\frac{m}{2\pi i \delta} \right)^{N/2} \int \prod_{j=1}^{N-1} dq_j \exp\left(i \frac{m}{2\delta} \left[\frac{(q_N - q_{N-1})^2 + (q_{N-1} - q_{N-2})^2}{+\dots (q_2 - q_1)^2 + (q_1 - q_0)^2} \right] \right)$$
(17.29)

where $q_0 = q$ and $q_N = q'$ are the initial and final points. The integrals are Gaussian and can be evaluated exactly, although the fact that they are coupled complicates matters significantly. The result is

$$K = \lim_{N \to \infty} \left(\frac{m}{2\pi i\delta}\right)^{N/2} \frac{1}{\sqrt{N}} \left(\frac{2\pi i\delta}{m}\right)^{(N-1)/2} e^{im(q'-q)^2/2N\delta}$$
$$= \lim_{N \to \infty} \left(\frac{m}{2\pi iN\delta}\right)^{1/2} e^{im(q'-q)^2/2N\delta}$$
(17.30)

But $N\delta$ is the total time interval T, so that we get

$$K = \left(\frac{m}{2\pi iT}\right)^{1/2} e^{im(q'-q)^2/2T}$$
(17.31)

in agreement with equation (17.28).

A couple of remarks are in order. First, we can write the argument of the exponential as

$$T \times \frac{1}{2}m\left(\frac{q'-q}{T}\right)^2 \tag{17.32}$$

which is just the action $S(q_{classical})$ for a particle moving along the classical path (a straight line in this case) between the initial and final points.

Secondly, we can restore the factors of \hbar if we want, by ensuring the correct dimensions. The argument of the exponential is the action, so in order to make it a pure number we must divide by \hbar . Furthermore, the propagator has the dimension of the inner product of two position eigenstates, which is inverse length. In order that the coefficient have this dimension we must multiply by $\hbar^{-1/2}$. The final result is

$$K = \left(\frac{m}{2\pi i\hbar T}\right)^{1/2} e^{iS(q_c)/\hbar} \tag{17.33}$$

This result typifies a couple of important features of calculations in this subject, which we will see repeatedly as we continue the discussion. First, the propagator separates into two factors, one which is the phase $e^{iS(q_c)/\hbar}$. Second, calculations in the PI formalism are typically quite a bit more lengthy than using standard techniques of quantum mechanics.

Harmonic Oscillator

As a second example of the computation of a PI, let us show how to compute the propagator for the harmonic oscillator using this method.

Let us start with the somewhat-formal version of the configuration-space PI (equation(17.25)):

$$K(q',T;q,0) = \int Dq(t) \exp(iS(q(t)))$$
(17.34)

For the harmonic oscillator

$$S(q(t)) = \int_{0}^{T} dt \left(\frac{1}{2}m\dot{q}^{2} - \frac{1}{2}m\omega^{2}q^{2}\right)$$
(17.35)

The paths over which the integral is to be performed go from q(0) = q to q(T) = q'. To do this PI, suppose we know the solution of the classical problem, $q_c(t)$:

$$\ddot{q}_c + \omega^2 q_c^2 = 0$$
 , $q_c(0) = q$, $q_c(T) = q'$ (17.36)

We can write $q(t) = q_c(t) + y(t)$ and perform a change of variables in the PI to y(t), since integrating over all deviations from the classical path is equivalent to integrating over all possible paths. Since at each time q and y differ by a constant, the Jacobian of the transformation is 1. Furthermore, since ? obeys the correct boundary conditions, the paths y(t) over which we integrate go from y(0) = 0 to y(T) = 0. The action for the path $q_c(t) + y(t)$ can be written as a power series in y:

$$S(q_{c}(t) + y(t)) = \int_{0}^{T} dt \left(\frac{1}{2}m\dot{q}_{c}^{2} - \frac{1}{2}m\omega^{2}q_{c}^{2}\right) + \underbrace{(linear\ in\ y)}_{=0} + \int_{0}^{T} dt \left(\frac{1}{2}m\dot{y}^{2} - \frac{1}{2}m\omega^{2}y^{2}\right) \quad (17.37)$$

The term linear in y vanishes by construction - q_c being the classical path, is the path for which the action is stationary! So we may write

$$S(q_c(t) + y(t)) = S(q_c(t)) + S(y(t))$$
(17.38)

We substitute this into equation (17.25) and obtain

$$K(q',T;q,0) = e^{iS(q_c(t))} \int Dq(t)e^{iS(y(t))}$$
(17.39)

As mentioned above, the paths y(t) over which we integrate go from y(0) = 0 to y(T) = 0. The only appearance of the initial and final positions is in the classical path, i.e., in the classical action. Once again, the PI separates into

two factors. The first is written in terms of the action of the classical path and the second is a PI over deviations from this classical path. The second factor is independent of the initial and final points.

This separation into a factor depending on the action of the classical path and a second one, a PI which is independent of the details of the classical path is a recurring theme and an important one. Indeed, it is often the first factor which contains most of the useful information contained in the propagator and it can be deduced without even performing a PI. It can be said that much of the work in the game of path integrals consists in avoiding having to compute one!

The evaluation of equation (17.39) is complicated and will be done at the end of this chapter. The result is

$$K(q',T;q,0) = \left(\frac{m\omega}{2\pi i \sin\left(\omega T\right)}\right)^{1/2} e^{iS(q_c(t))}$$
(17.40)

where

$$S(q_c(t)) = \frac{m\omega}{2\sin\left(\omega T\right)} \left(\left(q'^2 + q^2\right)\cos\left(\omega T\right) - 2q'q \right)$$
(17.41)

We close this section with two remarks. First, the PI for any quadratic action can be evaluated exactly (see derivation later), essentially since such a PI consists of Gaussian integrals. The general result is given later.

Second, K(q',T;q,0) is the amplitude to propagate from one point to another in a given time interval. Now we ask this question: if a particle is initially at position q, what is the wave function after the elapse of a time T? If we consider K as a function of the final position and time, it turns out to be the wave function for a particle with a specific initial condition and, as such, the propagator satisfies the Schrodinger equation at its final point.

17.4 The Classical Limit

17.4.1 "Derivation" of the Principle of Least Action

Since the example calculations performed above are somewhat dry and mathematical, it is worth backing up a bit and staring at the expression for the configuration space PI, equation(17.25):

$$K = \int Dq(t) \exp\left(iS(q(t))\right)$$

This innocent looking expression tells us something which is at first glance unbelievable and at second glance *really* unbelievable. The first glance observation is that a particle, in going from one position to another, takes all possible paths between these two positions. This is, if not actually unbelievable, at the very least counter-intuitive. We could, however, argue away much of what makes us feel uneasy if we could convince ourselves that while all paths contribute, the classical path is the dominant one.

However, the second glance observation is not reassuring. If we compare the contribution of the classical path (whose action is $S(q_c(t))$), with that of some other, arbitrarily wild, path (whose action is $S(q_w(t))$), we find that the first is $\exp(iS(q_c(t)))$ while the second is $\exp(iS(q_w(t)))$. They are both complex numbers of *unit magnitude* - each path taken in isolation is *equally important*. The classical path is no more important than any arbitrarily complicated path!

How are we to reconcile this *really* unbelievable conclusion with the fact that a ball thrown in the air has a more-or-less parabolic motion?

The key, not surprisingly, is in how the different paths interfere with one another. By considering the case where the rough scale of classical action is much bigger than the quantum of action, \hbar , we will see the emergence of the Principle of Least Action.

Consider two neighboring paths q(t) and q'(t) which contribute to the PI (see Figure 17.2 below).



Figure 17.2: Two Neighboring Paths

Let $q'(t) = q(t) + \eta(t)$, with $\eta(t)$ small. Then we can write the action as a functional Taylor expansion about the classical path.

If you are not familiar with the manipulation of functionals (functions of functions) do not despair - the only rule needed beyond standard calculus is the functional derivative

$$\frac{\delta q(t)}{\delta q(t')} = \delta(t - t') \tag{17.42}$$

where the last function is the Dirac delta function.

We have

$$S(q') = S(q+\eta) = S(q) + \int dt \eta(t) \frac{\delta S(q(t))}{\delta q(t)} + O(\eta^2)$$
(17.43)

The two paths contribute $\exp(iS(q(t)))$ and $\exp(iS(q'(t)))$ to the PI. The combined contribution is

$$A \simeq e^{iS(q)/\hbar} \left(1 + \exp\left(\frac{i}{\hbar} \int dt \eta(t) \frac{\delta S(q)}{\delta q(t)}\right) \right)$$
(17.44)

where we have neglected corrections of order η^2 . We see that the difference in phase between the two paths, which determines the interference between the two contributions, is

$$\frac{1}{\hbar} \int dt \eta(t) \frac{\delta S(q)}{\delta q(t)} \tag{17.45}$$

e see that the smaller the value of \hbar , the larger the phase difference between two given paths. So even if the paths are very close together, so that the difference in actions is extremely small, for sufficiently small \hbar the phase difference will still be large and on average destructive interference occurs.

This argument must be rethought, however, for one exceptional path - the path which extremizes the action, i.e., the classical path $q_c(t)$. For this path

$$S(q_c + \eta) = S(q_c) + O(\eta^2)$$
(17.46)

Thus, the classical path and a very close neighbor will have actions which differ by much less than two randomly chosen but equally close paths (see Figure 17.3 below).



Figure 17.3: Paths near classical path interfere constructively

This means that for fixed closeness of two paths and for fixed \hbar , paths near the classical path will on average interfere constructively (small phase difference) whereas for random paths the interference will be on average destructive.

Thus, heuristically, we conclude that is the problem is classical (action $\gg \hbar$), the most important contribution to the PI comes from the region around the path which extremizes the PI. In other words, the particle's motion is governed by the principle that the action is stationary. This, of course, is none other than the Principle of Least Action from which the Euler-Lagrange equations of classical mechanics are derived.

17.5 Topology and Path Integrals in Quantum Mechanics

In path integrals, if the configuration space has holes in it such that two paths between the same initial and final points are not deformable into one another, interesting effects can arise. This property of the configuration space goes by the following catchy name: non-simple-connectedness. We now study a situation of this type.

17.5.1 Aharonov-Bohm Effect

The Aharonov-Bohm effect (already discussed in Chapter 8) is one of the most dramatic illustrations of a purely quantum effect: the influence of the electromagnetic potential on particle motion even if the particle is *perfectly* shielded from any electric and magnetic fields. While classically the effect of electric and magnetic fields can be understood purely in terms of the forces these fields create on the particles, Aharonov and Bohm devised an ingenious thought experiment (which has since been carried out in the laboratory) showing that this is no longer true in quantum mechanics. Their effect is best illustrated by a refinement of Young's double-slit experiment, where particles passing through a barrier with two slits in it produce an interference pattern on a screen further downstream as shown in Figure 17.4 below.



Figure 17.4: Aharonov-Bohm effect. Magnetic flux is confined within the shaded area. particles are excluded from this area by a perfect shield

Aharonov and Bohm proposed that such an experiment be performed with charged particles. The setup had an added twist. A magnetic field from which the particles are perfectly shielded exists in between the two slits. If we perform the experiment first with no magnetic flux and then with a nonzero and arbitrary flux passing through the shielded region, the interference pattern will change, in spite of the fact that the particles are perfectly shielded from the magnetic field and feel no electric or magnetic force whatsoever.

Classically, we say - no force, no effect. Not so in quantum mechanics. PIs provide a excellent way of understanding this effect.

Consider first two representative paths $q_1(t)$ and $q_2(t)$ (in two dimensions) passing through slits 1 and 2 respectively, and which arrive at the same spot on the screen as shown in Figure 17.5 below.



Figure 17.5: Two representative paths contributing to the amplitude for a given point on the screen

Before turning on the magnetic field, let us suppose that the actions for these paths are $S(q_1)$ and $S(q_2)$. Then the interference of the amplitudes is determined by

$$e^{iS(q_1)/\hbar} + e^{iS(q_2)/\hbar} = e^{iS(q_1)/\hbar} \left(1 + e^{i(S(q_2) - S(q_1))/\hbar}\right)$$
(17.47)

The relative phase is

$$\varphi_{12} \equiv (S(q_2) - S(q_1))/\hbar$$
 (17.48)

Thus, the two paths interfere constructively if $\varphi_{12} = 2n\pi$ and destructively if $\varphi_{12} = (2n+1)\pi$ and, in general, there is partial cancellation between the two contributions.

How is this result affected if we add a magnetic field \vec{B} ? We can describe this field by a vector potential, writing $\vec{B} = \nabla \times \vec{A}$. This affects the particle's motion by the following change in the Lagrangian (see Chapter 8):

$$L(\vec{q}, \dot{\vec{q}}) \to L'(\vec{q}, \dot{\vec{q}}) = L(\vec{q}, \dot{\vec{q}}) - \frac{e}{c} \vec{v} \cdot \vec{A}(\vec{q})$$
(17.49)

Thus, the action changes by

$$-\frac{e}{c}\int dt\,\vec{v}\cdot\vec{A}(\vec{q}) = -\frac{e}{c}\int dt\,\frac{d\vec{q}(t)}{dt}\cdot\vec{A}(\vec{q}) = -\frac{e}{c}\int d\vec{q}(t)\cdot\vec{A}(\vec{q})$$

The integral is

$$\int d\vec{q}(t) \cdot \vec{A}(\vec{q}) \tag{17.50}$$

which is the line integral of \overline{A} long the path taken by the particle. So including the effect of the magnetic field, the action of the first path is

$$S'(\vec{q}_1) = S(\vec{q}_1) - \frac{e}{c} \int_{\vec{q}_1} d\vec{q}(t) \cdot \vec{A}(\vec{q})$$
(17.51)

and similarly for the second path.

Let us now look at the interference between the two paths, including the magnetic field.

$$e^{iS'(\vec{q}_1)/\hbar} + e^{iS'(\vec{q}_2)/\hbar} = e^{iS'(\vec{q}_1)/\hbar} \left(1 + e^{i(S'(\vec{q}_2) - S'(\vec{q}_1))/\hbar}\right) = e^{iS'(\vec{q}_1)/\hbar} \left(1 + e^{i\varphi'_{12}}\right)$$
(17.52)

where the new relative phase is

$$\varphi_{12}' = \varphi_{12} - \frac{e}{\hbar c} \left(\int_{\vec{q}_2} d\vec{q}(t) \cdot \vec{A}(\vec{q}) - \int_{\vec{q}_1} d\vec{q}(t) \cdot \vec{A}(\vec{q}) \right)$$
(17.53)

But the difference in the line integrals in equation (17.53) is a contour integral

$$\int_{\vec{q}_2} d\vec{q}(t) \cdot \vec{A}(\vec{q}) - \int_{\vec{q}_1} d\vec{q}(t) \cdot \vec{A}(\vec{q}) = \oint d\vec{q}(t) \cdot \vec{A}(\vec{q}) = \Phi$$
(17.54)

where Φ is the flux inside the closed loop bounded by the two paths. So we can write

$$\varphi_{12}' = \varphi_{12} - \frac{e\Phi}{\hbar c} \tag{17.55}$$

It is important to note that the change of relative phase due to the magnetic field is independent of the details of the two paths, as long as each passes through the corresponding slit. This means that the PI expression for the amplitude for the particle to reach a given point on the screen is affected by the magnetic field in a particularly clean way. Before the magnetic field is turned on, we may write $A = A_1 + A_2$, where

$$A_{1} = \int_{slit \ 1} D\vec{q} \, e^{iS'(\vec{q})/\hbar}$$
(17.56)

and similarly for A_2 . Including the magnetic field,

$$A_{1}' = \int_{slit \ 1} D\vec{q} \ e^{i(S'(\vec{q}) - \frac{e}{c} \int_{1}^{c} d\vec{q} \cdot \vec{A}/\hbar} = e^{-ie \int_{1}^{c} d\vec{q} \cdot \vec{A}/\hbar c} A_{1}$$
(17.57)

where we have pulled the line integral out of the PI since it is the same for all paths passing through slit 1 arriving at the point on the screen under consideration. So the amplitude is

$$A = e^{-ie \int_{1}^{d} d\vec{q} \cdot \vec{A} / hc} A_{1} + e^{-ie \int_{2}^{d} d\vec{q} \cdot \vec{A} / hc} A_{2} = e^{-ie \int_{1}^{d} d\vec{q} \cdot \vec{A} / hc} \left(A_{1} + e^{-ie \oint_{1}^{d} d\vec{q} \cdot \vec{A} / hc} A_{2} \right)$$
$$= e^{-ie \int_{1}^{d} d\vec{q} \cdot \vec{A} / hc} \left(A_{1} + e^{-ie \Phi / hc} A_{2} \right)$$
(17.58)

The overall phase is irrelevant and the interference pattern is influenced directly by the phase $e\Phi/\hbar c$. If we vary the phase continuously (by varying the magnetic flux), we can detect a shift in the interference pattern. For example, if $e\Phi/\hbar c = \pi$, then a spot on the screen which formerly corresponded to constructive interference will now be destructive and vice versa.

Since the interference is dependent only on the phase difference $mod(2\pi)$, as we vary the flux we get a shift of the interference pattern which is periodic, repeating itself when $e\Phi/hc$ changes by an integer times 2π .

17.6 Evaluation of Path Integrals - Details

We consider the case of particles moving in one dimension labelled by the position coordinate x. The particles have associated with them a Lagrangian

$$L(x, \dot{x}, t) = \frac{1}{2}m\dot{x}^2 - U(x)$$
(17.59)

In order to define the path integral we assume a series of times $t_N > t_{N-1} > t_{N-2} > \dots > t_1 > t_0$ letting N go to infinity later. The spacings between the times t + j + 1 and t_j will all be identical, namely

$$t_{j+1} - t_j = \frac{t_N - t_0}{N} = \varepsilon_N$$
 (17.60)

The discretization in time leads to a discretization of the paths x(t) which will be represented through the series of space-time points

$$\{(x_0, t_0), (x_1, t_1), (x_2, t_2), \dots, (x_{N-1}, t_{N-1}), (x_N, t_N)\}$$
(17.61)

Even though the time instances are fixed, we note that the x_j the values are not. They can be anywhere in the allowed volume which we will choose to be the interval $[-\infty, +\infty]$. In passing from one space-time instance (x_j, t_j) to the next (x_{j+1}, t_{j+1}) we assume that kinetic energy and potential energy are constant, namely,

$$\frac{1}{2}m\frac{(x_{j+1}-x_j)^2}{\varepsilon_N^2} \text{ and } U(x_j)$$
(17.62)

respectively. these assumptions lead then to the following Riemann form for the action integral

$$S[x(t)] = \lim_{N \to \infty} \varepsilon_N \sum_{j=0}^{N-1} \left(\frac{1}{2} m \frac{(x_{j+1} - x_j)^2}{\varepsilon_N^2} - U(x_j) \right)$$
(17.63)

where the form S[...] is the standard form for a *functional*.

The main idea is that one can replace the path integral now by a multiple

integral over x_1, x_2 , etc. This allows us to write the propagator or evolution operator as

$$K(x_N, t_N; x_0, t_0) = \lim_{N \to \infty} C_N \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \dots \int_{-\infty}^{\infty} dx_{N-1} \exp\left(\frac{i}{\hbar} \varepsilon_N \sum_{j=0}^{N-1} \left(\frac{1}{2}m \frac{(x_{j+1} - x_j)^2}{\varepsilon_N^2} - U(x_j)\right)\right)$$
(17.64)

Here, c_N is a constant which depends on N and other constants in the exponent. It needs to be chosen to make sure that the limit in equation(17.64) can be properly taken. Its value is

$$C_N = \left(\frac{m}{2\pi i \hbar \varepsilon_N}\right)^{N/2} \tag{17.65}$$

17.6.1 Propagator for a Free Particle

Rather then using the integration variables x_j , it is more suitable to define new integration variables y_j , the origin of which coincides with the classical path of the particle. To see the benefit of such an approach, we define a path y(t) as follows

$$x(t) = x_{cl}(t) + y(t)$$
(17.66)

where $x_{cl}(t)$ is the classical path which connects the space-time points (x_0, t_0) and (x_N, t_N) , namely,

$$x_{cl}(t) = x_0 + \frac{x_N - x_0}{t_N - t_0} (t - t_0)$$
(17.67)

It is essential for the following to note that, since $x(t_0) = x_{cl}(t_0) = x_0$ and $x(t_N) = x_{cl}(t_N) = x_N$, it holds that

$$y(t_0) = y(t_N) = 0 \tag{17.68}$$

Also we use the fact that the velocity of the classical path

$$\dot{x}_{cl} = \frac{x_N - x_0}{t_N - t_0} \tag{17.69}$$

is constant. The action integral $S[x(t)|x(t_0) = x_0, x(t_N) = x_N]$ for any path x(t) can be expressed through an action integral over the path y(t) relative to the classical path(note explicit new notation). We get

$$S[x(t)|x(t_0) = x_0, x(t_N) = x_N] = \int_{t_0}^{t_N} dt \frac{1}{2} m \left(\dot{x}_{cl}^2 + 2\dot{x}_{cl} \dot{y} + \dot{y}^2 \right)$$
$$= \frac{1}{2} m \int_{t_0}^{t_N} dt \, \dot{x}_{cl}^2 + m \dot{x}_{cl} \int_{t_0}^{t_N} dt \, \dot{y} + \frac{1}{2} m \int_{t_0}^{t_N} dt \, \dot{y}^2 \qquad (17.70)$$

The condition (17.68) implies for the second term on the RHS

$$\int_{t_0}^{t_N} dt \, \dot{y} = y(t_N) - y(t_0) = 0 \tag{17.71}$$

The first term on the RHS of (17.70) is using (17.67)

$$\frac{1}{2}m\int_{t_0}^{t_N} dt \, \dot{x}_{cl}^2 = \frac{1}{2}m\frac{\left(x_N - x_0\right)^2}{t_N - t_0} \tag{17.72}$$

The third term can be written in the notation introduced above

$$\frac{1}{2}m\int_{t_0}^{t_N} dt \, \dot{y}^2 = S[x(t)|x(t_0) = 0, x(t_N) = 0]$$
(17.73)

i.e., due to (17.68), can be expressed through a path integral with endpoints $x(t_0) = 0, x(t_N) = 0$. The resulting expression for $S[x(t)|x(t_0) = x_0, x(t_N) = x_N]$ is

$$S[x(t)|x(t_0) = x_0, x(t_N) = x_N]$$

= $\frac{1}{2}m\frac{(x_N - x_0)^2}{t_N - t_0} + S[x(t)|x(t_0) = 0, x(t_N) = 0]$ (17.74)

Inserting into the expression for the propagator we have

$$K(x_N, t_N; x_0, t_0) = \exp\left[\frac{im}{2\hbar} \frac{(x_N - x_0)^2}{t_N - t_0}\right]_{x(t_0) = 0}^{x(t_N) = 0} D[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right)$$
(17.75)

which can be written as

$$K(x_N, t_N; x_0, t_0) = \exp\left[\frac{im}{2\hbar} \frac{(x_N - x_0)^2}{t_N - t_0}\right] K(0, t_N; 0, t_0)$$
(17.76)

Thus, we need to evaluate

$$K(0,t_N;0,t_0) = \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \varepsilon_N}\right)^{N/2} \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \dots \int_{-\infty}^{\infty} dy_{N-1} \exp\left(\frac{i}{\hbar} \varepsilon_N \sum_{j=0}^{N-1} \left(\frac{1}{2} m \frac{(y_{j+1} - y_j)^2}{\varepsilon_N^2}\right)\right)$$
(17.77)

The exponent E can be written, using

$$E = \frac{im}{2\hbar\varepsilon_N} \begin{pmatrix} 2y_1^2 - y_1y_2 - y_2y_1 + 2y_2^2 - y_2y_3 - y_3y_2 \\ +2y_3^2 - \dots - y_{N-2}y_{N-1} - y_{N-1}y_{N-2} + 2y_{N-1}^2 \end{pmatrix}$$

$$= i\sum_{j,k=1}^{N-1} y_j a_{jk} y_k$$
(17.78)

where the a_{jk} are the elements of the following symmetric $(N-1) \times (N-1)$ matrix

The following integral

$$I = \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \dots \int_{-\infty}^{\infty} dy_{N-1} \exp\left(i \sum_{j,k=1}^{N-1} y_j a_{jk} y_k\right)$$
(17.80)

must now be determined. We will exploit the fact that for any real, symmetric matrix there exists a similarity transformation such that

$$S^{-1}aS = \begin{pmatrix} \tilde{a}_{11} & 0 & 0 & . & . & 0 & 0 \\ 0 & \tilde{a}_{22} & 0 & . & . & 0 & 0 \\ 0 & 0 & \tilde{a}_{33} & . & . & 0 & 0 \\ . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & \tilde{a}_{n-1,n-1} & 0 \\ 0 & 0 & 0 & . & . & 0 & \tilde{a}_{nn} \end{pmatrix}$$
(17.81)

where S can be chosen as an orthonormal transformation, i.e.,

$$S^T S = I \to S^T = S^{-1} \tag{17.82}$$

The \tilde{a}_{kk} are the eigenvalues of the a matrix and are real. This property allows us to simplify the bilinear form $\sum_{j,k}^{n} y_j a_{jk} y_k$ by introducing new integration variables

$$\tilde{y}_j = \sum_{k}^{n} \left(S^{-1} \right)_{jk} y_k \quad , \quad y_k = \sum_{k}^{n} S_{jk} \tilde{y}_k$$
(17.83)

The bilinear form then reads in terms of \tilde{y}_j

$$\sum_{j,k}^{n} y_j a_{jk} y_k = \sum_{j,k}^{n} \sum_{\ell,m}^{n} \tilde{y}_\ell S_{\ell j} a_{jk} S_{km} \tilde{y}_m = \sum_{j,k}^{n} \sum_{\ell,m}^{n} \tilde{y}_\ell \left(S^T\right)_{\ell j} a_{jk} S_{km} \tilde{y}_m = \sum_{j,k}^{n} \tilde{y}_j \tilde{a}_{jk} \tilde{y}_m$$

where we have used (from equations (17.81) and (17.82))

$$\tilde{a}_{jk} = \sum_{\ell,m}^{n} \left(S^T \right)_{j\ell} a_{\ell m} S_{mk} \tag{17.84}$$

For the determinant of \tilde{a} we have

$$\det(\tilde{a}) = \prod_{j=1}^{n} \tilde{a}_{jj} \tag{17.85}$$

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as well as

$$\det(\tilde{a}) = \det(S^{-1}aS) = \det(S^{-1})\det(a)\det(S) = \det(a) = \prod_{j=1}^{n} \tilde{a}_{jj}$$
(17.86)

We have assumed that $det(a) \neq 0$. Accordingly we have

$$\prod_{j=1}^{n} \tilde{a}_{jj} \neq 0 \tag{17.87}$$

so that none of the eigenvalues of a vanishes, i.e., $\tilde{a}_{jj} \neq 0$ for j = 1, 2, ..., n. Substitution of the integration variables (17.83) in equation(17.80) gives

$$I = \int_{-\infty}^{\infty} d\tilde{y}_1 \int_{-\infty}^{\infty} d\tilde{y}_2 \dots \int_{-\infty}^{\infty} d\tilde{y}_{N-1} \left| \det\left(\frac{\partial(y_1, \dots, y_n)}{\partial(\tilde{y}_1, \dots, \tilde{y}_n)}\right) \right| \exp\left(i\sum_{k=1}^{n} \tilde{a}_{kk}\tilde{y}_k^2\right) \quad (17.88)$$

where we have introduced the Jacobian matrix

$$J = \frac{\partial(y_1, \dots, y_n)}{\partial(\tilde{y}_1, \dots, \tilde{y}_n)} \tag{17.89}$$

with elements

$$J_{js} = \frac{\partial y_j}{\partial \tilde{y}_s} \tag{17.90}$$

According to equation (17.84), J = S and hence det(J) = 1. We then have

$$I = \int_{-\infty}^{\infty} d\tilde{y}_1 \int_{-\infty}^{\infty} d\tilde{y}_2 \dots \int_{-\infty}^{\infty} d\tilde{y}_{N-1} \exp\left(i\sum_{k}^{n} \tilde{a}_{kk} \tilde{y}_k^2\right)$$
$$= \int_{-\infty}^{\infty} d\tilde{y}_1 \exp\left(i\tilde{a}_{11} \tilde{y}_1^2\right) \dots \int_{-\infty}^{\infty} d\tilde{y}_n \exp\left(i\tilde{a}_{nn} \tilde{y}_n^2\right)$$
$$= \prod_{k=1-\infty}^{n} \int_{-\infty}^{\infty} d\tilde{y}_k \exp\left(i\tilde{a}_{kk} \tilde{y}_k^2\right)$$
(17.91)

which leaves us to determine integrals of the type

$$\int_{-\infty}^{\infty} dx \ e^{icx^2} \tag{17.92}$$

where $c \neq 0$. We first consider the case c > 0. One can relate the integral (17.92) to the standard Gaussian integral

$$\int_{-\infty}^{\infty} dx \ e^{-cx^2} = \sqrt{\frac{\pi}{c}} \ , \ c > 0$$
 (17.93)



Figure 17.6: Contour path in the complex plane

by considering the contour integral

$$J = \oint_{\gamma} dz \ e^{icz^2} \tag{17.94}$$

along the path $\gamma = \gamma_1 + \gamma_2 + \gamma_3 + \gamma_4$ shown in Figure 17.6 below.

The contour integral vanishes since e^{icz^2} is an analytic function, i.e., the integrand does not have any singularities anywhere inside the contour. The contour integral (17.94) can be written as the sum of the following path integrals

$$J = J_1 + J_2 + J_3 + J_4 \quad , \quad J_k = \oint_{\gamma_k} dz \ e^{icz^2}$$
(17.95)

The contributions J_k can be expressed through integrals along a real coordinate axis by realizing that the paths γ_k can be parameterized by real coordinates x

$$\gamma_1 : z = x$$
 $J_1 = \int_{-p}^{p} dx \ e^{icx^2}$ (17.96)

$$\gamma_2: z = ix + p$$
 $J_2 = \int_0^p i \, dx \, e^{ic(ix+p)^2}$ (17.97)

$$\gamma_3 : z = \sqrt{i} x \qquad J_3 = \int_{\sqrt{2}p}^{-\sqrt{2}p} \sqrt{i} \, dx \, e^{ic(\sqrt{i} \, x)^2} = -\sqrt{i} \int_{-\sqrt{2}p}^{\sqrt{2}p} dx \, e^{-cx^2} \qquad (17.98)$$

$$\gamma_4: z = ix - p$$
 $J_4 = \int_{-p}^{0} i \, dx \, e^{ic(ix-p)^2}$ (17.99)

for $x, p \in \mathfrak{R}$.

Substituting -x for x into integral J_4 we get

$$J_4 = \int_{p}^{0} (-i) \, dx \, e^{ic(-ix-p)^2} = \int_{0}^{p} i \, dx \, e^{ic(ix+p)^2} = J_2 \tag{17.100}$$

We now show that the two integrals J_2 and J_4 vanish for $p \to \infty$. This follows from the calculation below.

$$\lim_{p \to +\infty} |J_{2 \text{ or } 4}| = \lim_{p \to +\infty} \left| \int_{0}^{p} i \, dx \, e^{ic(ix+p)^{2}} \right| \le \lim_{p \to +\infty} \left| \int_{0}^{p} |i| \, dx \, \left| e^{ic(p^{2}-x^{2})} \right| \left| e^{-2cxp} \right| \right|$$
$$\lim_{p \to +\infty} |J_{2 \text{ or } 4}| \le \lim_{p \to +\infty} \left| \int_{0}^{p} dx \, \left| e^{-2cxp} \right| \right| = \lim_{p \to +\infty} \frac{1 - e^{-2cp}}{2cp} = 0$$

Therefore, J_2 and J_4 do not contribute to the integral (17.95) for $p \to \infty$. We then have

$$\int_{-\infty}^{\infty} dx \ e^{icx^2} = \sqrt{i} \int_{-\infty}^{\infty} dx \ e^{-cx^2} = \sqrt{\frac{i\pi}{c}}$$
(17.101)

One can derive the same result for c<0, if one chooses the same contour but with a path γ that is reflected at the real axis. This gives

$$J = \int_{-\infty}^{\infty} dx \ e^{icx^2} - \sqrt{-i} \int_{-\infty}^{\infty} dx \ e^{cx^2} = 0 \qquad , \quad c < 0$$
$$\int_{-\infty}^{\infty} dx \ e^{icx^2} = \sqrt{\frac{-i\pi}{-|c|}} = \sqrt{\frac{i\pi}{c}} \qquad (17.102)$$

Putting everything together we have

$$I = \prod_{k=1}^{n} \sqrt{\frac{i\pi}{\tilde{a}_{kk}}} = \sqrt{\frac{(i\pi)^n}{\prod\limits_{k=1}^{n} \tilde{a}_{kk}}} = \sqrt{\frac{(i\pi)^n}{\det(a)}}$$
(17.103)

This last result holds for a d-dimensional real, symmetric matrix (a_{jk}) with $det(a_{jk}) \neq 0$. In order to complete the evaluation of the propagator in equation(17.64) we split off the factor $m/2\hbar\varepsilon_N$ in the definition (17.79) of (a_{jk}) defining a new matrix (A_{jk}) through

$$a_{jk} = \frac{m}{2\hbar\varepsilon_N} A_{jk} \tag{17.104}$$

Using

$$\det(a_{jk}) = \left(\frac{m}{2\hbar\varepsilon_N}\right)^{N-1} \det(A_{jk})$$
(17.105)

which is a general property of determinants, we get

$$K(0,t_N;0,t_0) = \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \varepsilon_N}\right)^{N/2} \left(\frac{2\pi i \hbar \varepsilon_N}{m}\right)^{(N-1)/2} \frac{1}{\sqrt{\det(A_{jk})}}$$
(17.106)

In order to determine $det(A_{jk})$ we consider the dimension n of (A_{jk}) , presently N-1, as a variable and let $n = 1, 2, \ldots$. We seek to evaluate the determinant of the $n \times n$ matrix

For this purpose, we expand (17.107) in terms of subdeterminants along the last column. One can readily verify that this procedure leads to the following recursion equation for the determinants

$$D_n = 2D_{n-1} - D_{n-2} \tag{17.108}$$

To solve this three term recursion relationship one needs two starting values. Using

$$D_1 = \det(2) = 2$$
 , $D_2 = \det\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} = 3$ (17.109)

we get

$$D_n = n + 1 \tag{17.110}$$

Therefore, we get

$$\det(A_{jk}) = N \tag{17.111}$$

which gives

$$K(0, t_N; 0, t_0) = \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \varepsilon_N N} \right)^{1/2} = \left(\frac{m}{2\pi i \hbar (t_N - t_0)} \right)^{1/2}$$
(17.112)

and from (17.76)

$$K(x,t;x_0,t_0) = \left(\frac{m}{2\pi i\hbar(t-t_0)}\right)^{1/2} \exp\left(\frac{im}{2\hbar}\frac{(x-x_0)^2}{t-t_0}\right)$$
(17.113)

which agrees with our earlier result (17.33).

The propagator allows us to predict the time evolution of any state function $\psi(x,t)$ of a free particle. The result can be generalized to three dimensions as

$$K(\vec{r},t;\vec{r}_0,t_0) = \left(\frac{m}{2\pi i\hbar(t-t_0)}\right)^{3/2} \exp\left(\frac{im}{2\hbar}\frac{(\vec{r}-\vec{r}_0)^2}{t-t_0}\right)$$
(17.114)

17.6.2 Propagator for a Quadratic Lagrangian

We now need to develop equations to reproduce the result for a harmonic oscillator in equations (17.40 and (17.41)).

We want to determine the propagator

$$K(x_N, t_N; x_0, t_0) = \int_{x(t_0)=x_0}^{x(t_N)=x_N} D[x(t)] \exp\left(\frac{i}{\hbar}S[x(t)]\right)$$
(17.115)

for the quadratic Lagrangian

$$L(x, \dot{x}, t) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}c(t)x^2 - e(t)x$$
(17.116)

We need to determine the action integral

$$S[x(t)] = \int_{t_0}^{t_N} dt' L(x, \dot{x}, t')$$
(17.117)

for an arbitrary path x(t) with end points $x(t_0) = x_0$ and $x(t_N) = x_N$. In order to simplify this task we again define a new path y(t)

$$x(t) = x_{cl}(t) + y(t)$$
(17.118)

which describes the deviation from the classical path $x_{cl}(t)$ with end points $x(t_0) = x_0$ and $x(t_N) = x_N$ so that

$$y(t_0) = y(t_N) = 0 \tag{17.119}$$

This gives

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$$L(x_{cl} + y, \dot{x}_{cl} + \dot{y}, t) = L(x_{cl}, \dot{x}_{cl}, t) + L'(y, \dot{y}(t), t) + \delta L$$
(17.120)

where

$$L(x_{cl}, \dot{x}_{cl}, t) = \frac{1}{2}m\dot{x}_{cl}^2 - \frac{1}{2}c(t)x_{cl}^2 - e(t)x_{cl}$$
(17.121)

$$L'(y, \dot{y}(t), t) = \frac{1}{2}m\dot{y}^2 - \frac{1}{2}c(t)y^2 - e(t)y$$
(17.122)

$$\delta L = m\dot{x}_{cl}\dot{y}(t) - c(t)x_{cl}y - e(t)y \qquad (17.123)$$

We now show that the contribution of δL to the action integral (17.117) vanishes. For this purpose we use

$$\dot{x}_{cl}\dot{y} = \frac{d}{dt}\left(\dot{x}_{cl}y\right) - \ddot{x}_{cl}y \tag{17.124}$$

and get

$$\int_{t_0}^{t_N} dt \delta L = m \left(\dot{x}_{cl} y \right) \Big|_{t_0}^{t_N} - \int_{t_0}^{t_N} dt \left[m \ddot{x}_{cl}(t) + c(t) x_{cl}(t) + e(t) \right] y(t)$$
(17.125)

According to (17.119) the first term on the RHS vanishes. Getting the Euler-Lagrange equations from the Lagrangian (17.116) we have for the classical path

$$m\ddot{x}_{cl}(t) + c(t)x_{cl}(t) + e(t) = 0$$
(17.126)

and hence, the second term on the RHS also vanishes. Thus,

$$\int_{t_0}^{t_N} dt \delta L = 0$$
 (17.127)

We then have

$$K(x_N, t_N; x_0, t_0) = \exp\left(\frac{i}{\hbar}S[x_{cl}(t)]\right)\tilde{K}(0, t_N; 0, t_0)$$
(17.128)

where

$$\tilde{K}(0,t_N;0,t_0) = \int_{x(t_0)=x_0}^{x(t_N)=x_N} D[y(t)] \exp\left(\frac{i}{\hbar} \int_{t_0}^{t_N} dt \ L'(y,\dot{y},t)\right)$$
(17.129)

For the quadratic Lagrangian, we have achieved a separation in terms of a classical action integral and a propagator connecting the end points $y(t_0) = 0$ and $y(t_N) = 0$ which is analogous to the result (17.76). A similar discretization scheme gives in this case

$$\tilde{K}(0,t_N;0,t_0) = \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \varepsilon_N}\right)^{N/2} \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \dots \int_{-\infty}^{\infty} dy_{N-1} \exp\left(\frac{i\varepsilon_N}{\hbar} \sum_{j=0}^{N-1} \left(\frac{m(y_{j+1}-y_j)^2}{2\varepsilon_N^2} - \frac{c_j y_j^2}{2}\right)\right)$$
(17.130)

where $c_j = c(t_j)$, $t_j = t_0 + \varepsilon_N j$. Again, we can write the exponent in (17.130) using a quadratic form

$$E = i \sum_{j,k=1}^{N-1} y_j a_{jk} y_k \tag{17.131}$$

where the a_{jk} are the elements of the following symmetric $(N-1) \times (N-1)$ matrix

$$(a_{jk}) = \frac{m}{2\hbar\varepsilon_N} \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \vdots & 2 & -1 \\ 0 & 0 & 0 & \vdots & 2 & -1 \\ 0 & 0 & 0 & \vdots & -1 & 2 \end{pmatrix}$$

$$-\frac{\varepsilon_N}{2\hbar} \begin{pmatrix} c_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & c_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & c_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \vdots & \vdots & c_{N-1} \end{pmatrix}$$
(17.132)

In the case, det $(a_{jk}) \neq 0$, we can express the multiple integral in (17.130) using (17.103) as

$$\tilde{K}(0,t_N;0,t_0) = \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \varepsilon_N}\right)^{N/2} \left(\frac{(i\pi)^{N-1}}{\det(a)}\right)^{1/2}$$
$$= \lim_{N \to \infty} \left[\frac{m}{2\pi i \hbar} \frac{1}{\varepsilon_N \left(\frac{2\hbar \varepsilon_N}{m}\right)^{N-1} \det(a)}\right]^{1/2}$$
(17.133)

Therefore we need to evaluate the function

$$f(t_0, t_N) = \lim_{N \to \infty} \left[\varepsilon_N \left(\frac{2h\varepsilon_N}{m} \right)^{N-1} \det(a) \right]$$
(17.134)

According to (17.132) we have

$$D_{N-1} \stackrel{def}{=} \left(\frac{2\hbar\varepsilon_N}{m}\right)^{N-1} \det(a)$$

$$= \frac{m}{2\hbar\varepsilon_N} \begin{pmatrix} 2 - \frac{\varepsilon_N^2}{m}c_1 & -1 & 0 & . & 0 & 0 \\ -1 & 2 - \frac{\varepsilon_N^2}{m}c_2 & -1 & . & 0 & 0 \\ 0 & -1 & 2 - \frac{\varepsilon_N^2}{m}c_3 & . & 0 & 0 \\ . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & 2 - \frac{\varepsilon_N^2}{m}c_{N-2} & -1 \\ 0 & 0 & 0 & . & . & -1 & 2 - \frac{\varepsilon_N^2}{m}c_{N-1} \end{pmatrix}$$

In the following we will assume that the dimension n = N - 1 of the matrix is a variable (as in the earlier derivation). One can then derive a recursion

relationship for the D_n

$$D_{n} = \left(2 - \frac{\varepsilon_{N}^{2}}{m}c_{n}\right)D_{n-1} - D_{n-2}$$
(17.136)

using the method of expanding a determinant in terms of subdeterminants as earlier. Using the starting values

$$D_0 = 1 ; D_1 = \left(2 - \frac{\varepsilon_N^2}{m}c_1\right)$$
 (17.137)

this recursion relationship can be used to determine D_{n-1} . We can write (17.136) as a 2nd-order difference equation

$$\frac{D_{n+1} - 2D_n + D_{n-1}}{\varepsilon_N^2} = -\frac{c_{N+1}D_n}{m}$$
(17.138)

Since we are interested in the solution of this equation in the limit of vanishing ε_N we can interpret (17.138) as a 2nd-order differential equation in the continuous variable $t = n\varepsilon_N + t_0$

$$\frac{d^2 f(t_0, t)}{dt^2} = -\frac{c(t)}{m} f(t_0, t)$$
(17.139)

The boundary conditions at $t = t_0$ (according to (17.137)) are

$$f(t_0, t_0) = \varepsilon_N D_0 = 0 \tag{17.140}$$

$$\left. \frac{df(t_0,t)}{dt} \right|_{t=t_0} = \varepsilon_N \frac{D_1 - D_0}{\varepsilon_N} = 2 - \frac{\varepsilon_N^2}{m} c_1 - 1 = 1 - \frac{\varepsilon_N^2}{m} c_1 = 1$$
(17.141)

We finally get for the propagator (17.115)

$$K(x,t;x_0,t_0) = \left(\frac{m}{2\pi i \hbar f(t_0,t)}\right)^{1/2} \exp\left(\frac{i}{\hbar} S[x_{cl}(t)]\right)$$
(17.142)

where $f(t_0, t)$ is the solution of ((17.139)-(17.141)) and where $S[x_{cl}(t)]$ is determined by first solving the Euler-Lagrange equations for the Lagrangian (17.116)to obtain the classical path $x_{cl}(t)$ with end points $x_{cl}(t_0) = x_0$ and $x_{cl}(t_N) = x_N$ and then evaluating (17.117) for this path. Note that the required solution $x_{cl}(t)$ involves a solution of the Euler-Lagrange equations for boundary condition which are different from those conventionally encountered in Classical Mechanics where we usually find a solution for initial conditions $x_{cl}(t_0) = x_0$ and $\dot{x}_{cl}(t_0) = v_0$.

17.6.3 Propagator of a Harmonic Oscillator

In order to illustrate the evaluation of (17.142) we consider the case of a harmonic oscillator (we just quoted the result of the calculation earlier). In this case, the coefficients in the Lagrangian (17.116) are $c(t) = m\omega^2$ and e(t) = 0, i.e., the Lagrangian is

$$L(x, \dot{x}, t) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2$$
(17.143)

We first determine $f(t_0, t)$. In this case we have

$$\ddot{f} = -\omega^2 f$$
 , $f(t_0, t_0) = 0$, $\dot{f}(t_0, t_0) = 1$ (17.144)

The solution which obeys these boundary conditions is

$$f(t_0, t) = \frac{\sin \omega (t - t_0)}{\omega}$$
 (17.145)

We now determine $S[x_{cl}(t)]$. For this purpose we first find the path $x_{cl}(t)$ which obeys $x_{cl}(t_0) = x_0$ and $x_{cl}(t) = x$ and satisfies the Euler-Lagrange equation for the harmonic oscillator

$$m\ddot{x}_{cl} + m\omega^2 x_{cl}^2 = 0 \Rightarrow x_{cl}(\tau) = A\sin\omega(\tau - t_0) + B\cos\omega(\tau - t_0)$$
(17.146)

Imposing the boundary conditions gives

$$B = x_0 \quad , \quad A = \frac{x - x_0 \cos \omega (t - t_0)}{\sin \omega (t - t_0)} \tag{17.147}$$

and the desired path is

$$x_{cl}(\tau) = \frac{x - x_0 c}{s} \sin \omega (\tau - t_0) + x_0 \cos \omega (\tau - t_0)$$
(17.148)

where we have introduced the notation

$$c = \cos \omega (t - t_0)$$
 , $s = \sin \omega (t - t_0)$ (17.149)

We now determine the action integral associated with the path ((17.148), (17.149))

$$S[x_{cl}(t)] = \int_{t_0}^{t} d\tau \left(\frac{1}{2}m\dot{x}_{cl}^2(\tau) - \frac{1}{2}m\omega^2 x_{cl}^2(\tau)\right)$$
(17.150)

We assume that $t_0 = 0$. From (17.148) the velocity along the classical path is

$$\dot{x}_{cl}(\tau) = \omega \frac{x - x_0 c}{s} \sin \omega \tau - \omega x_0 \cos \omega \tau \qquad (17.151)$$

and for the kinetic energy we get

$$\frac{m}{2}\dot{x}_{cl}^{2}(\tau) = \frac{m\omega^{2}}{2}\frac{(x-x_{0}c)^{2}}{s^{2}}\cos^{2}\omega\tau -m\omega^{2}x_{0}\frac{x-x_{0}c}{s}\cos\omega\tau\sin\omega\tau + \frac{m\omega^{2}x_{0}^{2}}{2}\sin^{2}\omega\tau$$
(17.152)

Similarly, we get the potential energy

$$\frac{m\omega^2}{2}x_{cl}^2(\tau) = \frac{m\omega^2}{2}\frac{(x-x_0c)^2}{s^2}\sin^2\omega\tau - m\omega^2x_0\frac{x-x_0c}{s}\cos\omega\tau\sin\omega\tau + \frac{m\omega^2x_0^2}{2}\cos^2\omega\tau \qquad (17.153)$$

Using

$$\cos^{2}\omega\tau = \frac{1}{2} + \frac{1}{2}\cos 2\omega\tau \quad , \quad \sin^{2}\omega\tau = \frac{1}{2} - \frac{1}{2}\cos 2\omega\tau \qquad (17.154)$$

$$\cos\omega\tau\sin\omega\tau = \frac{1}{2}\sin2\omega\tau \tag{17.155}$$

the Lagrangian, considered as a function of τ , reads

$$g(\tau) = \frac{1}{2}m\dot{x}_{cl}^{2}(\tau) - \frac{1}{2}m\omega^{2}x_{cl}^{2}(\tau)$$
$$= \frac{m\omega^{2}}{2}\left(\frac{(x - x_{0}c)^{2}}{s^{2}} - x_{0}^{2}\right)\cos 2\omega\tau - m\omega^{2}\sin 2\omega\tau \qquad (17.156)$$

Evaluation of the action integral

$$S[x_{cl}(t)] = \int_{0}^{t} d\tau g(\tau)$$
 (17.157)

requires the integrals

$$\int_{0}^{t} d\tau \cos 2\omega \tau = \frac{\sin 2\omega \tau}{2\omega} = \frac{sc}{\omega} \quad , \quad \int_{0}^{t} d\tau \sin 2\omega \tau = \frac{1 - \cos 2\omega \tau}{2\omega} = \frac{s^{2}}{\omega} \quad (17.158)$$

where we have used the definitions (17.149). We finally get

$$S[x_{cl}(t)] = \frac{m\omega}{2\sin\omega(t-t_0)} \left[\left(x_0^2 + x^2 \right) \cos\omega(t-t_0) - 2x_0 x \right]$$
(17.159)

The expression for the propagator of the harmonic oscillator is then given by

$$K(x,t;x_0,t_0) = \left(\frac{m\omega}{2\pi i\hbar\sin\omega(t-t_0)}\right)^{1/2} \exp\left(\frac{im\omega}{2\hbar\sin\omega(t-t_0)}\left[\left(x_0^2+x^2\right)\cos\omega(t-t_0)-2x_0x\right]\right)\right)$$
(17.160)

17.7 Problems

17.7.1 Path integral for a charged particle moving on a plane in the presence of a perpendicular magnetic field

Consider a particle of mass m and charge e moving on a plane in the presence of an external uniform magnetic field perpendicular to the plane and with strength

B. Let $\vec{r} = (x_1, x_2)$ and $\vec{p} = (p_1, p_2)$ represent the components of the coordinate \vec{r} and of the momentum \vec{p} of the particle. The Lagrangian for the particle is

$$L = \frac{1}{2}m\left(\frac{d\vec{r}}{dt}\right)^2 + \frac{e}{c}\frac{d\vec{r}}{dt} \cdot \vec{A}(\vec{r})$$

- 1. Find the relation between the momentum \vec{p} and the coordinate \vec{r} and explain how the momentum is related to the velocity $\vec{v} = d\vec{r}/dt$ in this case.
- 2. Show that the classical Hamiltonian of for this problem is

$$H(q,p) = \frac{1}{2m} \left(\vec{p}^2 - \frac{e}{c} \vec{A}(\vec{r}) \right)^2$$

where $\vec{A}(\vec{r})$ is the vector potential for a uniform magnetic field, normal to the plane, and of magnitude *B*. In what follows, we will always write the vector potential in the gauge $\nabla \cdot \vec{A}(\vec{r}) = 0$, where it is given by

$$A_1(\vec{r}) = -\frac{B}{2}x_2$$
 , $A_2(\vec{r}) = \frac{B}{2}x_1$

- 3. Use canonical quantization to find the quantum mechanical Hamiltonian and the commutation relations for the observables.
- 4. Derive the form of the *path integral*, as a sum over the histories of the position $\vec{r}(t)$ of the particle, for the transition amplitude of the process in which the particle returns to its initial location \vec{r}_0 at time t_f having left that point at t_i , i.e.,

$$\langle \vec{r}_0, t_f | \vec{r}_0, t_i \rangle$$

where \vec{r}_0 is an arbitrary point of the plain and $|t_f - t_i| \to \infty$. What is the form of the action? What initial and final conditions should be satisfied by the histories $\vec{r}(t)$?

17.7.2 Path integral for the three-dimensional harmonic oscillator

Consider a harmonic oscillator of mass m and frequency ω in three dimensions. We will denote the position vector of the oscillator by $\vec{r} = (x, y, z)$. The classical Hamiltonian is

$$H(\vec{r},\vec{p}) = \frac{\vec{p}^2}{2m} + \frac{1}{2}m\omega^2\vec{r}^2$$

Derive an expression for the path integral for the matrix element

$$\langle \vec{r}_f = 0, t_f \, | \, \vec{r}_i = 0, t_i \rangle$$

for this three-dimensional oscillator, where $t_f \to +\infty$ and $t_i \to -\infty$. Make sure you explain how this limit is taken. HINT: you will find it convenient to write the path integral in terms of the histories of the three components x(t), y(t)and z(t).

17.7.3 Transitions in the forced one-dimensional oscillator

Consider a one-dimensional oscillator of mass m and frequency ω , labeled by the coordinate q(t) on an infinite line. The oscillator is subject to an external force J(t) of the form

$$J(t) = W \frac{\tau}{t^2 + \tau^2}$$

- 1. What are the units of W? Use W and m to construct a quantity with units of energy.
- 2. Using path integral methods calculate the amplitude

$$\langle q=0, t_f \mid q=0, t_i \rangle$$

for $t_i \to -\infty$ and $t_f \to +\infty$.

- 3. How does the expression you found depend on W, τ , m and ω ? Give a physical interpretation to this dependence by looking at the extreme regimes of τ large and small (relative to what?).
- 4. What dependence on W would you have expected to find in the Born approximation? And in higher orders in perturbation theory?

17.7.4 Green's Function for a Free Particle

The Green's function for the single-particle Schrodinger equation is defined as the solution of the equation

$$\left[i\hbar\partial_t - \hat{H}\right]G(\vec{r},t;\vec{r}',t') = i\hbar\delta(t-t')\delta(\vec{r}-vecr')$$

Find explicitly the expression for the green's function, $G_0(t - t', \vec{r} - \vec{r}')$, of a free particle in one and two spatial dimensions in *real space-time representation*. HINT: Use the Fourier transform to solve the above equation. Shift the pole in the Green's function, $G(\varepsilon, \vec{p})$, $(\epsilon \to \epsilon + i0)$ and use the inverse Fourier transform to obtain the representation of interest.

17.7.5 Propagator for a Free Particle

The single-particle propagator that appears in the derivation of the Feynman path integral is defined as the solution of the equation:

$$\left[i\hbar\partial_t - \hat{H}\right]K(x,t;x_i,t_i) = i\hbar\delta(t-t_i)\delta(x-x_i)$$

which is to be complemented with the initial condition:

$$K(x,t+0;x_i,t_i) = \delta(x-x_i)$$

We have derived the following path integral expression for the propagator:

$$K(x,t;x_i,t_i) = \mathcal{N} \int [\mathcal{D}x(t)] exp\left(\frac{i}{\hbar}S[x(t)]\right)$$

where \mathcal{N} is a normalization constant and S is the classical action understood as a functional of x(t).

Using the above definition of the path integral, calculate explicitly the propagator for a free particle in one spatial dimension. Compare your result with that of Problem 17.7.4.

Chapter 18

Solid State Physics

18.1 Crystal Structure and Symmetry

Crystalline solids are regular periodic arrays of atoms and are characterized by having long-range spatial order. The periodicity of crystals and the resultant high symmetry makes it easier to study these systems.

We will use the Born-Oppenheimer approximation scheme we used earlier with molecules. In this case, we assume that the motion of the electrons in the solid can be dealt with separately from that of the nuclei.

The nuclear part of the problem involves several types of motion. For a solid with N nuclei and hence 3N nuclear degrees of freedom we have

- 1. Translation of the solid as a whole (3 degrees of freedom). This is motion of the center of mass of the entire crystal.
- 2. Rotation of the solid as a whole (3 degrees of freedom). This is *rigid-body* rotation of the crystal (no nuclear motion) about the center of mass.
- 3. Vibration of the nuclei in the solid (3N 6 degrees of freedom). This motion is called *lattice vibrations*.

To study the electron motions in the crystal, we ignore the lattice vibrations and the motion of the crystal as a whole. We assume that the nuclei are fixed at their equilibrium positions (*the crystal*). The electronic Schrödinger equation is then

$$\hat{H}'\psi^e_{\varepsilon}(\vec{r}_i;\vec{R}_{\alpha}) = E^e_{\varepsilon}\psi^e_{\varepsilon}(\vec{r}_i;\vec{R}_{\alpha})$$
(18.1)

where

$$\begin{split} \hat{H}' &= \hat{T}_e + \hat{V}_{ee} + \hat{V}_{en} \end{split} \tag{18.2}$$

$$\hat{T}_e &= \text{electron kinetic energy} \\
\hat{V}_{ee} &= \text{electron - electroninteraction} , \quad \hat{V}_{en} &= \text{electron - nucleus interaction} \\
\psi^e_{\varepsilon}(\vec{r}_i; \vec{R}_{\alpha}) &= \text{electron wavefunctions} \\
E^e_{\varepsilon} &= \text{electron energies} \\
\vec{r}_i &= \text{electroncoordinates} , \quad \vec{R}_{\alpha} &= \text{nuclear coordinates} \end{split}$$

Although we can formally write these equations, we have a problem. The solid contains a very large number of electrons (and nuclei), i.e., for a solid $1 \ cm^3$ in volume we have on the order of 10^{23} electrons, which leads to an enormous number of coupled equations. We cannot solve these equations.

We will use a *one-electron approach* to this multielectron system. We assume the so-called orbital approximation where we write the full electronic wave function in terms of single-particle wave functions. This means that we approximate the electron-electron interaction terms in the Hamiltonian with a smooth average potential, which reflects the periodicity of the crystal. It turns out that the details of the approximation are not crucial as long as the periodicity is accurately incorporated. This approach leads eventually to the band theory of solids. Real crystals are extraordinarily complicated environments which make the study of crystals very difficult. They are finite so that there are surface effects and they contain defects and impurities which destroy the symmetry of the crystal structure. While these complications lead to interesting effects, they are not important for the study of the energy level structure. We will assume *ideal* crystals, i.e., we confine our attention to regions deep inside the crystal so that we can neglect surface effects. These are called *bulk regions* and their properties are independent of any surface details. Essentially, we are assume that the crystals are infinite in extent. We also assume that the crystals are pure and without defects so that the crystal symmetry is perfect. Finally, we only include electrostatic terms in the Hamiltonian. We will restrict our attention to those features of the crystal structure and associated symmetry that are needed to study the electronic energy level structure.

18.1.1 Symmetry of the Crystal System

A symmetry operation is a coordinate transformation that leaves the system unchanged or *invariant*. In crystals, we say that the system and the associated Hamiltonian are invariant under some symmetry operations. Symmetry operations provide a scheme for classifying crystal structures and , in addition, will give us a powerful method for determining the energy level structures.
Translational Symmetry

A crystal(ideal) has translational symmetry. This means that we can pick it up and move it through a specified vector and we cannot distinguish the final crystal from the original. For example, we consider a one-dimensional crystal as shown in Figure 18.1 below.



Figure 18.1: 1-dimensional crystal

In the one-dimensional crystal, which extends the entire length $[-\infty, +\infty]$ of the x-axis, each atom is separated from its nearest neighbor by a distance d. The choice of origin is arbitrary. If we translate the crystal in either direction by an amount nd where n = 1, 2, 3, ... the resulting crystal is indistinguishable from the original. The crystal is then said to have *translational symmetry* and the vectors

$$\vec{T} = n\hat{e}_x , \quad n = \pm 1, \pm 2, \dots$$
(18.3)

are called *lattice translation vectors*. The word *lattice* as used here refers to the set of mathematical points which characterize the translational symmetry of the crystal.

We say that two points on the are equivalent if the surrounding crystal looks the same independent of which of the two points we *stand on*. Clearly, any two such points must be connected by a lattice translation vector. The points do not have to be lattice points.

We generalize to 3- (or 2-) dimensions by defining the general translation vector as

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c} \tag{18.4}$$

where

 n_1, n_2, n_3 are any integers

 \vec{a} , \vec{b} , \vec{c} are any 3 noncoplanar lattice translation vectors in the crystal

All of these vectors are defined with respect to some origin(arbitrary). This is illustrated for a 2-dimensional crystal in Figure 18.2 below.



Figure 18.2: 2-dimensional crystal

In Figure 18.3 below, translational invariance means that the interactions felt by an electron at position $\vec{r} + \vec{T}$ are identical to those felt at position \vec{r} .



Figure 18.3: Translation Invariance

The statement of translational invariance of the crystal in terms of the Hamiltonian operator means that

$$\hat{H}(\vec{r} + \vec{T}) = \hat{H}(\vec{r})$$
 (18.5)

The choice of the three vectors \vec{a} , \vec{b} and \vec{c} is not unique. In Figure 18.4 below we illustrate several choices (all equally good).



Figure 18.4: Alternate Basis Vectors

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The vector pairs (\vec{a}, \vec{b}) and (\vec{a}', \vec{b}') are primitive lattice translation vectors(not unique). The appellation primitive is attached because using the pair as a basis we can reach all lattice points. On the other hand the pair (\vec{a}'', \vec{b}'') are not primitive since a point like P cannot be reached.

The *lattice*, which is the set of all mathematical points that are equivalent under translation by $\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$ where \vec{a}, \vec{b} and \vec{c} are primitive lattice translation vectors, defines the structure of the crystal. The crystal consists of *lattice* + *basis*, where a *basis* is one or more atoms that are attached to *all* the lattice points.

As we have seen, the choice of basis is arbitrary. Sometimes one chooses a region of the crystal as the basis, where the region chosen can be *stacked* to generate the entire crystal. Such a region is called a *unit cell*. In Figure 18.4 above, the three sets of basis vectors each define a unit cell (a parallelogram in 2 dimensions).

A more detailed definition goes as follows: A volume of the crystal that when translated through all translation vectors, just fills all of space without either overlapping itself or leaving any gaps is called a *primitive cell or primitive unit cell*. It must contain exactly one lattice point. In Figure 18.4 above, (\vec{a}, \vec{b}) and (\vec{a}', \vec{b}') generate primitive unit cells, but (\vec{a}'', \vec{b}'') does not (it contains two atoms).

In addition, every primitive cell has the same area (volume). In Figure 18.5 below we have drawn several unit cells for a *rectangular-centered* lattice. The cells labelled (a), (b), and (d) are primitive while (c) is not.



Figure 18.5: Primitive Cells

Point Symmetry

There are another group of symmetry operations for a crystal which leave one point fixed in space. They are called *point symmetry operations*. The three most important point symmetry operations are rotation(R), reflection(F) and inversion(V). Not all crystal structures are characterized by all of these operations. In fact, they can be used to classify lattices and crystals.

Digression to Group Theory

A group is a set of elements A, B, C, ... such that a *group multiplication* is defined which associates a third element with any ordered pair of two elements. The multiplication must satisfy these requirements:

- 1. The product of any two elements in the set is in the set also, i.e., the set is *closed* under group multiplication.
- 2. The associative law holds, i.e., A(BC) = (AB)C.
- 3. There exists an identity element E such that EA = AE = A for any element A.
- 4. There exists an inverse A^{-1} for every element in the group, i.e., $AA^{-1} = A^{-1}A = E$.

The *order* of the group is equal to the number of elements.

An example is the set of four elements (group of order 4) with the multiplication table below

| | E | A | B | C |
|---|---|---|---|---|
| E | E | A | B | C |
| A | A | E | C | B |
| B | B | C | E | A |
| C | C | B | A | E |

Table 18.1: Group with 4 elements

If group multiplication is *commutative*, i.e., AB = BA for any pair of elements, then the group is *Abelian*. The above table represents a 4 element Abelian group.

Another example is the non-Abelian group of order 6 (6 elements) given by the table below

If the group multiplication operation were ordinary matrix multiplication, then a representation of this group (an explicit set of elements) is given by

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
$$B = \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \quad C = \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$$
$$D = \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}, \quad F = \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$$

| | E | A | B | C | D | F |
|---|---|---|---|---|---|---|
| E | E | A | B | C | D | F |
| A | A | E | D | F | В | C |
| B | B | F | E | D | C | A |
| C | C | D | F | E | A | B |
| D | D | C | A | B | F | E |
| F | F | B | C | A | E | D |

Table 18.2: Group with 6 elements

Notice that each row/column only contains each element once. This is an example of the rearrangement theorem, which says

In the sequence EA_k , A_1A_k , A_2A_k , A_3A_k ,, A_kA_k , each group element A_j appears exactly once (as one of the products). The elements are merely rearranged by multiplying each by A_j .

Returning to point symmetries, we first consider the 1–dimensional crystal, which is particularly simple. Its point symmetry operations form an Abelian group of order 2 given by

| | E | F |
|---|---|---|
| E | E | F |
| F | F | E |

Table 18.3: Abelian group of order 2

In this case, the two elements are

$$\begin{split} E &= identity \rightarrow does \ nothing \\ F &= reflection \rightarrow takes \ x \rightarrow -x \end{split}$$

In 2 dimensions, the possible point symmetry operations are

- 1. The identity operation.
- 2. Reflection through a *mirror* line in the plane of the crystal.
- 3. An *n*-fold rotation (through angle $2\pi/n$) about an axis perpendicular to the plane of the crystal where n = 2, 3, 4, or6.

Notice that n = 5 is not allowed. The symmetry elements corresponding to these operations are the mirror line and the n-fold axes (inversion is equivalent to a twofold rotation).

In 3 dimensions, the possible point symmetry operations are

- 1. The identity operation.
- 2. Reflection through one or more "*mirror* planes.
- 3. An *n*-fold rotation about an axis where n = 2, 3, 4, or 6.
- 4. Inversion through a center of symmetry $(\vec{r} \rightarrow -\vec{r})$.

The last operation, inversion, is actually equivalent to a rotation by π followed by reflection through a plane perpendicular to the axis of rotation. Because, of its importance, however, we keep it as a separate symmetry operation.

Since each point symmetry operation is a coordinate transformation, when we say that the crystal has a particular symmetry element (e.g., a center of symmetry), we mean that the corresponding symmetry operation (e.g., inversion) leaves the Hamiltonian of the crystal unchanged.

Classification of Two-Dimensional Lattices and Crystals

Lattices having different sets of point symmetries are labelled as distinct *Bravais* lattices. We can understand what distinguishes Bravais lattices using 2–dimensional lattices as an example. In two dimensions there are 5 Bravais lattices:

the oblique lattice, the primitive rectangular lattice, the centered rectangular lattice, the square lattice, and the hexagonal lattice.

The *oblique lattice* is the Bravais lattice of lowest symmetry. It is shown in Figure 18.6 below:



Figure 18.6: Oblique Lattice

The only symmetry operations for this lattice is twofold rotations about axes perpendicular to the plane of the crystal and passing through each lattice point and about axes halfway between each pair of lattice points as shown above. The primitive lattice translation vectors \vec{a} and \vec{b} have no simple relationship to each other. Each of the other four Bravais lattices are special cases of the oblique lattice. Each has more symmetry operations than the oblique lattice and, in each, the primitive lattice translation vectors \vec{a} and \vec{b} have some definite relationships.

The *primitive rectangular lattice* shown in Figure 18.7 below has the same twofold rotation axes as the oblique lattice and in addition has several mirror line as shown. Reflection through mirror lines is a symmetry operation of



Figure 18.7: Primitive Rectangular Lattice

the lattice. The primitive lattice translation vectors \vec{a} and \vec{b} are orthogonal to each other and their lengths are unrelated.

Another type of *rectangular lattice* is the *centered rectangular lattice* shown in Figure 18.8 below.



Figure 18.8: Centered Rectangular Lattice

This lattice has the twofold rotation axes, mirror lines and glide lines as shown.

A glide line is a symmetry element corresponding to a *combined* operation: to get from one point in the crystal to an equivalent point via a glide line, we first reflect across the glide line, and then translate along the glide line by 1/2 the repeat distance of the crystal. The angle between the lattice translation vector is as shown and their lengths are unrelated.

The square lattice is a special case of the primitive rectangular lattice where $|\vec{a}| = |\vec{b}|$. It is shown in Figure 18.9 below. In addition to the twofold rotation



Figure 18.9: Square Lattice

axes, mirror lines and glide lines of the primitive rectangular lattice, the square lattice has the fourfold rotation axes as shown in the diagram. The primitive lattice translation vectors are orthogonal and equal in length.

The *hexagonal lattice* is derived from the centered rectangular lattice by setting $|\vec{a}| = |\vec{b}|$ as shown in in Figure 18.10 below. This lattice has twofold , threefold and sixfold axes of rotation as shown. It has a large number of mirror line and glide lines as shown. The primitive lattice translation vectors are of equal length and make an angle of 60° with respect to each other.



Figure 18.10: Hexagonal Lattice

Symmetry of the Crystal

Up to this point we have dealt exclusively with the classification of lattices according to their *point symmetry*. As we stated earlier, however, a crystal is composed of a *lattice plus a basis* at each lattice point. Because of the basis, the point symmetry of the crystal may not be the same as that of the lattice, i.e., the symmetry of the crystal may be *lower* than that of the lattice. The lattice may possess some symmetry elements not possessed by the crystal. This is a very important point. Let us illustrate it with an example.

We consider a square lattice and, in particular, we look at the mirror lines through a lattice point as shown in Figure 18.11 below.



Figure 18.11: Mirror Lines in Square Lattice

Reflection through any of these mirror lines yields a lattice that is indistinguishable from the original lattice.

Now associating with each lattice point of this square lattice one of the two different *bases* as shown in Figure 18.12 below



Figure 18.12: Possible Bases

we get the crystals shown in Figure 18.13 below.



Figure 18.13: Possible Crystals

It is clear that the crystal on left possesses all of the same mirror lines as the original square lattice while the crystal on the right does not. The symmetry of the crystal on the right is *lower* than that of its lattice.

Three-Dimensional Crystals

Our discussions will mostly involve one- and two-dimensional crystals. Threedimensional crystals are significantly more difficult to study and we will only say some general things about them at the end.

In three dimensions there are 14 Bravais lattices. Three examples are shown in Figure 18.14 below.



Figure 18.14: 3-Dimensional Crystals

From each Bravais lattice we can construct crystals by associating a basis with each lattice point.

Miller Indices

In order to discuss three dimensional crystals we need to be able to specify particular directions (axes) and particular planes in the crystal.

A convention has been developed for dealing with this problem. Axes and planes in a crystal are described by *Miller indices*.

For example, to specify a particular axis in a crystal, we first write a lattice translation vector

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c} \tag{18.6}$$

that points along this axis. We then determine any integer factor N common to n_1 , n_2 and n_3 .

The Miller indices of the axis are then given by the set of integers

$$\left[\frac{n_1}{N}, \frac{n_2}{N}, \frac{n_3}{N}\right] = [h, k, l]$$
(18.7)

where negative indices are denoted by a bar over the integer.

An example is shown below for the body diagonal of a cubic lattice where

$$\vec{T} = \vec{a} + \vec{b} + \vec{c} \to N = 1 \to [1, 1, 1]$$
 (18.8)

as shown in Figure 18.15 below.



Figure 18.15: [111] axis in cubic lattice

To specify a particular plane in a crystal, we first determine the intercepts of the plane on three noncoplanar lattice translation vectors \vec{a} , \vec{b} and \vec{c} and call these intercepts a, b and c.

We then form the *reciprocals* of these intercepts. Finally, we *multiply* these

reciprocals by a common factor that reduces them to the three smallest integers. These are the Miller indices of the plane, written (h, k, l). Some examples are shown in Figure 18.16 below.



Figure 18.16: [111] axis in cubic lattice

A slightly more complicated example is one where the intercepts are (3, 4, 12)

so that

$$(a,b,c) = (3,4,12) \rightarrow \left(\frac{1}{3}, \frac{1}{4}, \frac{1}{12}\right) \times 12 = (4,3,1) = (h,k,l)$$
 (18.9)

The Miller indices for an axis represent all equivalent axes (all parallel). The Miller indices for a plane represent all equivalent planes (all parallel).

This concludes our short introduction to crystal structure and symmetry. The symmetry of the crystal is important beyond what it tells us about the classification of the crystal. It reflects the fundamental properties of the crystal Hamiltonian and in particular, the crystal potential energy. We will use these properties to deduce facts about the energy eigenfunctions for the electrons in the crystal.

18.2 Bloch Theorem, the Reciprocal Lattice and Brillouin Zones

We first study the general properties of electron wavefunctions in crystals that are a consequence of the periodicity of the crystal.

The electronic Schrodinger equation for a single electron in the crystal is given by

$$H\psi_E(\vec{r}) = E\psi_E(\vec{r}) \tag{18.10}$$

In the orbital approximation, the potential energy of the electron consists of terms describing its interaction with the static array of nuclei and average potential energy terms that take into account interactions with the other electrons in the crystal. The interaction potential with the nuclei clearly has the periodicity of the crystal and we assume that the average potential energy is constructed so that it also has the periodicity of the crystal. This means that the total potential energy is invariant under translation, i.e.,

$$\hat{V}(\vec{r} + \vec{T}) = \hat{V}(\vec{r})$$
 (18.11)

for any lattice translation vector \vec{T} . Since the kinetic energy operator is also translation invariant we then have

$$\hat{H}(\vec{r} + \vec{T}) = \hat{H}(\vec{r})$$
 (18.12)

i.e., the electronic Hamiltonian is invariant under translations.

18.2.1 Translation Operators in Configuration Space

We now introduce the translation operator \hat{T}_{op} which we define by its action on any function $f(\vec{r})$ as

$$\hat{T}_{op}f(\vec{r}) = f(\vec{r} + \vec{T})$$
 (18.13)

Each lattice translation vector $\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$ has a corresponding translation operator $\hat{T}_{op} = \hat{T}_{op}(n_1, n_2, n_3)$.

We define the *product* of two translation operators by the relation

$$\hat{T}'_{op}\hat{T}_{op}f(\vec{r}) = \hat{T}'_{op}f(\vec{r}+\vec{T}) = f(\vec{r}+\vec{T}+\vec{T}') = \hat{T}''_{op}f(\vec{r})$$
(18.14)

i.e., the product of two translation operators is another translation operator given by *successive* application of the two operators. \hat{T}''_{op} corresponds to the translation $\vec{T} + \vec{T}'$. This means that

$$\hat{T}_{op}(n_1, n_2, n_3)\hat{T}'_{op}(n'_1, n'_2, n'_3) = \hat{T}''_{op}(n_1 + n'_1, n_2 + n'_2, n_3 + n'_3)$$
(18.15)

$$\vec{T}^{\prime\prime} = \vec{T} + \vec{T}^{\prime} = (n_1 + n_1^{\prime})\vec{a} + (n_2 + n_2^{\prime})\vec{b} + (n_3 + n_3^{\prime})\vec{c}$$
(18.16)

This result will have important consequences later.

The invariance of \hat{H} under translation by any lattice translation vector \vec{T} is expressed by the commutator relation

$$\left[\hat{H}, \hat{T}_{op}\right] = 0$$
 (18.17)

for any \hat{T}_{op} . In addition, from the definition we can see that

$$\hat{T}'_{op}\hat{T}_{op} = \hat{T}_{op}\hat{T}'_{op} \tag{18.18}$$

i.e., the order of application is unimportant. This gives another commutator relation

$$\left[\hat{T}_{op}, \hat{T}'_{op}\right] = 0 \tag{18.19}$$

These commutators say that the set of operators $(\hat{H}, \{\hat{T}_{op}\})$ not only form a closed commutator algebra but also that the Hamiltonian \hat{H} and all lattice translation operators \hat{T}_{op} are a set of mutually commuting operators. This means that we can find a set of simultaneous eigenfunctions for all these operators. If we assume that ψ_E is a particular non-degenerate eigenfunction we can write the eigenvalue equation

$$\hat{T}_{op}\psi_E = \gamma\psi_E = \gamma(n_1, n_2, n_3)\psi_E$$
 (18.20)

where γ is a constant (the eigenvalue). This property of the energy eigenfunctions is a *direct consequence* of the translational invariance of the crystal.

What can we say about the constant γ ?

18.2.2 Derivation of Bloch's Theorem

All the energy eigenfunctions are normalized so that

$$\int |\psi_E(\vec{r})|^2 d^3r = 1$$
 (18.21)

This says that the eigenfunction

$$\psi_E(\vec{r} + \vec{T}) = \hat{T}_{op}\psi_E(\vec{r}) = \gamma\psi_E(\vec{r})$$
(18.22)

must satisfy

$$\int |\psi_E(\vec{r} + \vec{T})|^2 d^3r = |\gamma|^2 \int |\psi_E(\vec{r})|^2 d^3r = |\gamma|^2 = 1$$
(18.23)

Thus, we can always write $\gamma = e^{i\beta}$ where $\beta = \beta(n_1, n_2, n_3)$ is a constant. There is one γ (or β) corresponding to *each* lattice translation vector \hat{T} .

Applying successive translation operators we find that

$$\hat{T}'_{op}\hat{T}_{op}\psi_E(\vec{r}) = \hat{T}'_{op}\gamma\psi_E(\vec{r}) = \gamma'\gamma\psi_E(\vec{r})$$
$$= \hat{T}''_{op}\psi_E(\vec{r}) = \gamma''\psi_E(\vec{r})$$
(18.24)

$$\gamma'' = \gamma' \gamma \to e^{i\beta''} = e^{i\beta'} e^{i\beta} \to \beta(n_1, n_2, n_3) + \beta'(n_1', n_2', n_3') = \beta''(n_1 + n_1', n_2 + n_2', n_3 + n_3')$$
(18.25)

i.e., not only is β'' the sum of β' and β but also the arguments of β'' are the sum of the arguments of β' and β .

This says that we must have $\beta(n_1, n_2, n_3) = k_1n_1 + k_2n_2 + k_3n_3$, i.e., linear in all of its arguments $(k_1, k_2 \text{ and } k_3 \text{ are constants})$. This, in turn, says that β is proportional to \vec{T} , i.e., $\beta = \vec{k} \cdot \vec{T}$, where \vec{k} is a constant vector that is not depend on n_1, n_2 or n_3 . We can then write for the eigenvalue of the translation operator

$$\gamma = e^{i\beta} = e^{i\vec{k}\cdot\vec{T}} \tag{18.26}$$

and the eigenvalue equation takes the form

$$\hat{T}_{op}\psi_E(\vec{r}) = \psi_E(\vec{r} + \vec{T}) = \gamma\psi_E(\vec{r}) = e^{ik\cdot\vec{T}}\psi_E(\vec{r})$$
 (18.27)

This is Bloch's theorem of the first form.

It tells us that we can choose solutions of the Schrodinger equation such that for every Hamiltonian eigenfunction $\psi_E(\vec{r})$ there exists a vector \vec{k} called a *wave vector*, such that (18.27) holds for any translation operator \hat{T}_{op} , that is, that $\psi_E(\vec{r} + \vec{T})$ differs from $\psi_E(\vec{r})$ only by a multiplicative phase factor $e^{i\vec{k}\cdot\vec{T}}$. Any function that satisfies Bloch's theorem is called a *Bloch function or Bloch wave*.

Bloch's theorem is a direct consequence of the translational symmetry of the crystal.

The Wave Vector

The proportionality constant \vec{k} has units of inverse length. For each Hamiltonian eigenfunction $\psi_E(\vec{r})$, there is a wave vector \vec{k} . The relationship of \vec{k} to the wave function is given by Bloch's theorem. This means that \vec{k} can be viewed as a *quantum number* for the function $\psi_E(\vec{r})$ and we can write $\psi_{E,\vec{k}}(\vec{r})$.

What are some of the properties of the wave vector \vec{k} ?

We first consider the one-dimensional version of Bloch's theorem. Suppose that we have a one-dimensional crystal with equally spaced *atoms* (separation distance = d). We ask for the relation ship between $\psi_E(\vec{r})$ and k for a wave function of the form

$$\psi_E(x) = e^{i\alpha x} \tag{18.28}$$

where α is a real constant. In this case, Bloch's theorem becomes

$$\psi_E(x+nd) = e^{i\alpha(x+nd)} = e^{i\alpha nd} e^{i\alpha x} = e^{i\alpha nd} \psi_E(x) = e^{iknd} \psi_E(x)$$
(18.29)

It is clear that Bloch's theorem is satisfied for an infinite set of k-values given by

$$k = \alpha + \frac{2\pi}{d}m$$
, $m = 0, \pm 1, \pm 2, \dots$ (18.30)

where we have used the fact that $e^{i2\pi m} = 1$. This suggests that we cannot uniquely define the wave vector \vec{k} , i.e., there are an infinite number of wave vectors that are *equivalent* to each other in the way that they are related to the wave function $\psi_E(x)$. This result generalizes to three dimensions. For each single-particle Hamiltonian eigenfunction $\psi_E(\vec{r})$ we can find a set of different wave vectors \vec{k} that impose a similar restriction on $\psi_E(\vec{r})$, i.e., for which

$$\psi_E(\vec{r} + \vec{T}) = e^{ik \cdot T} \psi_E(\vec{r}) \tag{18.31}$$

In general, we choose the smallest of these wave vectors to label the eigenfunction $\psi_{E,\vec{k}}(\vec{r})$.

Alternative Form of Bloch's Theorem

We define a new function by

$$u_{E,\vec{k}}(\vec{r}) = e^{-i\vec{k}\cdot\vec{r}}\psi_{E,\vec{k}}(\vec{r})$$
(18.32)

Now from the definition of the translation operator we have

$$\hat{T}_{op}u_{E,\vec{k}}(\vec{r}) = u_{E,\vec{k}}(\vec{r}+\vec{T}) = e^{-i\vec{k}\cdot(\vec{r}+\vec{T})}\psi_{E,\vec{k}}(\vec{r}+\vec{T})$$
(18.33)

Using Bloch's theorem we get

$$\hat{T}_{op}u_{E,\vec{k}}(\vec{r}) = e^{-i\vec{k}\cdot(\vec{r}+\vec{T})}e^{i\vec{k}\cdot\vec{T}}\psi_{E,\vec{k}}(\vec{r}) = e^{-i\vec{k}\cdot\vec{r}}\psi_{E,\vec{k}}(\vec{r}) = u_{E,\vec{k}}(\vec{r})$$
(18.34)

This says that the new function $u_{E,\vec{k}}(\vec{r})$ is a periodic function invariant under translation by \vec{T} , i.e., it has the periodicity of the crystal. Using this result we rewrite the Hamiltonian eigenfunction as

$$\psi_{E,\vec{k}}(\vec{r}) = e^{ik\cdot\vec{r}} u_{E,\vec{k}}(\vec{r}) \tag{18.35}$$

which is the *second form* of Bloch's theorem. This form shows that the electronic eigenfunction of the crystal can be chosen to have the form of a periodic function $u_{E,\vec{k}}(\vec{r})$ modulated by a plane-wave envelope $e^{i\vec{k}\cdot\vec{r}}$.

Generally, this envelope varies more slowly with \vec{r} then does $u_{E,\vec{k}}(\vec{r})$. The real part of $\psi_{E,\vec{k}}(\vec{r})$ is shown in Figure 18.17 below, where it has been assumed that $u_{E,\vec{k}}(\vec{r})$ is a real function.



Figure 18.17: Second form of Bloch function

We have determined the qualitative form of the Hamiltonian eigenfunction for any crystal using only translational symmetry of the crystal. Bloch's theorem in the first form links the wave function and the wave vector and in the second form describes an important property of the wave function.

The Reciprocal Lattice

The strangest feature of Bloch's theorem is the proportionality constant \vec{k} . The name (wave vector) and the symbol (\vec{k}) used for this vector suggest(in analogy with the wave vector for free electrons) that \vec{k} will be related to the energy. This is, in fact, true as we shall show during the rest of this chapter. At this point, however, we will just label the energy eigenfunctions by both energy and wave vector.

Up to this point we have not restricted the magnitude of \vec{k} in any way. Thus,

there exists a continuum of values of \vec{k} . We call this continuum \vec{k} -space or reciprocal space.

Each vector in k-space has three components, in general, and we write

$$k = k_x \hat{x} + k_y \hat{y} + k_z \hat{z} \tag{18.36}$$

where \hat{x} , \hat{y} and \hat{z} are mutually orthogonal unit vectors in *regular or coordinate or direct space*. The crystal exists in direct space and its lattice is called the *direct lattice*. A lattice constructed in reciprocal space is called a *reciprocal lattice*.

Reciprocal Lattice Vectors

What do we mean precisely by the term reciprocal lattice?

Each crystal lattice in direct space has an associated reciprocal lattice in \bar{k} -space. Bloch's theorem says that for a particular energy eigenfunction of the electronic Hamiltonian, there exists a vector \vec{k} (actually an infinity of such vectors) such that

$$\hat{T}_{op}\psi_{E,\vec{k}}(\vec{r}) = \hat{T}_{op}e^{i\vec{k}\cdot\vec{r}}u_{E,\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot(\vec{r}+\vec{T})}u_{E,\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{T}}\psi_{E,\vec{k}}(\vec{r})$$
(18.37)

We now consider a vector, say \vec{G} , that satisfies the condition

$$e^{i\vec{G}\cdot\vec{T}} = 1 \tag{18.38}$$

i.e., \vec{G} is a *special* wave vector such that $u_{E,\vec{k}}(\vec{r})$ is invariant under any translation \hat{T}_{op} . The condition implies

$$e^{i\vec{G}\cdot\vec{T}} = \cos(\vec{G}\cdot\vec{T}) + i\sin(\vec{G}\cdot\vec{T}) = 1 \rightarrow \vec{G}\cdot\vec{T} = 2\pi n \quad , \quad n = \text{integer} \quad (18.39)$$

or that

$$\vec{G} \cdot \vec{T} = n_1 \vec{G} \cdot \vec{a} + n_2 \vec{G} \cdot \vec{b} + n_3 \vec{G} \cdot \vec{c} = 2\pi n \tag{18.40}$$

The integers n_1 , n_2 and n_3 which define a particular \vec{T} , can take on any values. For each set $\{n_1, n_2, n_3\}$ there exists some integer n for which the above equality holds. Thus, n depends on n_1 , n_2 and n_3 .

For example, suppose that $n_2 = 0$, $n_3 = 0$ and n_1 some arbitrary nonzero integer. Then we have

$$n_1 \vec{G} \cdot \vec{a} = 2\pi n \to \vec{G} \cdot \vec{a} = 2\pi n_a \tag{18.41}$$

since the relation must be valid for any value of n_1 . n_1 is another integer given by $n = n_a n_1$. Similarly, we must have

$$\vec{G} \cdot \vec{b} = 2\pi n_b \text{ and } \vec{G} \cdot \vec{c} = 2\pi n_c \tag{18.42}$$

These three relations allow us to write a general form for \vec{G}

$$\vec{G} = n_a \vec{A} + n_b \vec{B} + n_c \vec{C} \tag{18.43}$$

Although this looks like the expression for \vec{T} , remember, however, that \vec{G} is a vector in \vec{k} -space, i.e., that it is a vector such that

$$e^{i\vec{G}\cdot\vec{T}} = 1 \tag{18.44}$$

Putting everything together we get the relations

$$\begin{split} A \cdot \vec{a} &= 2\pi \quad , \quad B \cdot \vec{a} = 0 \quad , \quad C \cdot \vec{a} = 0 \\ \vec{A} \cdot \vec{b} &= 0 \quad , \quad \vec{B} \cdot \vec{b} = 2\pi \quad , \quad \vec{C} \cdot \vec{b} = 0 \\ \vec{A} \cdot \vec{c} &= 0 \quad , \quad \vec{B} \cdot \vec{c} = 0 \quad , \quad \vec{C} \cdot \vec{c} = 2\pi \end{split}$$

The first column of relations say that \vec{A} is orthogonal to both \vec{b} and \vec{c} or that we can write

$$\vec{A} = \eta_A \vec{b} \times \vec{c} \tag{18.45}$$

and

$$\vec{A} \cdot \vec{a} = 2\pi = \eta_A \vec{a} \cdot (\vec{b} \times \vec{c}) \tag{18.46}$$

so that

$$\vec{A} = 2\pi \frac{b \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \tag{18.47}$$

Similarly,

$$\vec{B} = 2\pi \frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \quad , \quad \vec{C} = 2\pi \frac{\vec{a} \times b}{\vec{a} \cdot (\vec{b} \times \vec{c})} \tag{18.48}$$

The three vectors \vec{A} , \vec{B} and \vec{C} are the primitive reciprocal lattice translation vectors. Used together with $\vec{G} = n_a \vec{A} + n_b \vec{B} + n_c \vec{C}$ (the reciprocal lattice translation vector) they generate a lattice of points in \vec{k} -space, called the reciprocal lattice. By construction, we see that each reciprocal lattice is defined with respect to a particular direct lattice(given by \vec{a} , \vec{b} and \vec{c}) in coordinate space.

Since $e^{i\vec{G}\cdot\vec{T}} = 1$, all vectors $\vec{k}' = \vec{k} + \vec{G}$ are equivalent in \vec{k} -space, i.e.,

$$e^{i\vec{k}'\cdot\vec{T}} = e^{i(\vec{k}+\vec{G})\cdot\vec{T}} = e^{i\vec{k}\cdot\vec{T}}e^{i\vec{G}\cdot\vec{T}} = e^{i\vec{k}\cdot\vec{T}}$$
(18.49)

There are an infinite number of such equivalent wave vectors where

$$\psi_{E,\vec{k}'}(\vec{r}+\vec{T}) = e^{ik'\cdot\vec{T}}\psi_{E,\vec{k}'}(\vec{r})$$
(18.50)

The Reciprocal Lattice for a Square Direct Lattice

We consider a crystal with a square direct lattice as shown inn Figure 18.18 below.

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where $|\vec{a}| = |\vec{b}|$. We have

$$\vec{a} = d\hat{x} \text{ and } b = d\hat{y} \tag{18.51}$$



Figure 18.18: Square direct lattice

The vector defining the reciprocal lattice in two dimensions is

$$\vec{G} = n_a \vec{A} + n_b \vec{B} \tag{18.52}$$

In order to calculate expressions for \vec{A} and \vec{B} in terms of \vec{a} and \vec{b} , the primitive lattice translation vectors of the square direct lattice, we temporarily introduce a third vector of the same length $\vec{c} = d\hat{z}$. This vector, which is orthogonal to the plane of the direct lattice, is only a mathematical tool useful for the stated purpose. Its properties will not enter the final answers.

We then have

$$\vec{a} \cdot (\vec{b} \times \vec{c}) = d^3$$
, $\vec{b} \times \vec{c} = d^2 \hat{x}$, $\vec{c} \times \vec{a} = d^2 \hat{y}$ (18.53)

so that

$$\vec{A} = \frac{2\pi}{d}\hat{x} \quad , \quad \vec{B} = \frac{2\pi}{d}\hat{y} \tag{18.54}$$

This result shows that the reciprocal lattice of a square direct lattice is also a square lattice with the spacing of adjacent lattice points in the x and y direction given by $2\pi/d$.

This is, in fact, a general property of two-dimensional Bravais lattices. They are *self-reciprocal*, i.e., the reciprocal lattice of a particular two-dimensional Bravais lattice is another lattice of the same Bravais type.

The reciprocal lattice is shown in Figure 18.19 below.

Some Other Properties

The reciprocal lattice of a particular direct lattice is unique, i.e., it is independent of the choice of primitive lattice translation vectors. We note that, if we



Figure 18.19: Reciprocal Lattice for Square direct lattice

start with a particular direct lattice in coordinate space, construct from it the reciprocal lattice in \vec{k} -space, and then construct the reciprocal of the reciprocal lattice, we obtain the original direct lattice in coordinate space.

Brillouin Zones Made Simple

The reciprocal lattice is a periodic array of mathematical points in \vec{k} -space, where each point is defined by a lattice translation vector \vec{G} . Because of its relationship to the electronic wave function $\psi_{E,\vec{k}}(\vec{r})$ via Bloch's theorem, each vector \vec{k} even if it is not a \vec{G} vector, is important.

As we noted earlier, a particular \vec{k} vector is not unique. The infinity of vectors $\vec{k}' = \vec{k} + \vec{G}$ are all equivalent for each vector \vec{k} .

We choose to label the wave functions by the *smallest* or *most significant* vector in each of the sets of equivalent vectors.

We now ask the following question: Is there a particular region of the reciprocal lattice that contains all of the *significant* \vec{k} vectors for a particular crystal?

The First Brillouin Zone

Since \vec{k} is the smallest vector in the set $\{\vec{k}' = \vec{k} + \vec{G}\}$, we know that

$$|\vec{k}'| \ge |\vec{k}|$$
 for any \vec{k}' in $\{\vec{k}' = \vec{k} + \vec{G}\}$ (18.55)

Consider the two different wave vectors \vec{k}_1 and \vec{k}_2 for a particular two-dimensional crystal shown in Figure 18.20 and Figure 18.21 below. We also show the vectors

$$\vec{k}_1' = \vec{k}_1 - \vec{G} \text{ and } \vec{k}_2' = \vec{k}_2 - \vec{G}$$
 (18.56)

where \vec{G} is a particular reciprocal lattice vector for the crystal. In the Figure



Figure 18.20: $|\vec{k}_1'| > |\vec{k}_1|$

18.20 above, $|\vec{k}_1'| > |\vec{k}_1|$ and in Figure 18.21 below $|\vec{k}_1'| > |\vec{k}_1|$. Thus, \vec{k}_1 may be the



smallest vector in its set, but \vec{k}_2 is certainly not the smallest vector in its set.

One difference between \vec{k}_1 and \vec{k}_2 is that the tip of \vec{k}_1 lies to the left of the perpendicular bisector of \vec{G} , whereas the tip of \vec{k}_2 lies to the right of the bisector.

It turns out that any wave vector whose tip lies on the side of the bisector away from the origin, is equivalent to at least one smaller wave vector, which can be generated by subtracting the lattice vector that was bisected. All the *significant* wave vectors (i.e., those not equivalent to some smaller wave vector), lie on the side of the perpendicular bisector closest to the origin.

Now, suppose that instead of bisecting one reciprocal lattice vector \vec{G} , we bisect all such vectors from the origin to nearby points. Then these bisectors enclose a

particular region of reciprocal space that includes the origin. Figure 18.22 below gives this construction for the square lattice(in reciprocal space) The enclosed



Figure 18.22: Construction of first zone

region (shaded) is called the *first Brillouin zone*. The solid arrows are lattice vectors and the dotted lines are their bisectors.

Each vector in the first Brillouin zone is the smallest vector in the set of equivalent vectors since it lies on the side toward the origin of every perpendicular bisector of \vec{G} . Any vector whose tip lies outside the first zone is equivalent to some smaller vector whose tip is inside the first zone. The first Brillouin zone contains all \vec{k} -values closer to the origin than any other point of the reciprocal lattice.

Higher Brillouin Zones

The \bar{k} -values inside the first Brillouin zone have special significance. We will generally restrict our attention to these values and ignore the infinity of other vectors outside this zone. Each vector outside the first Brillouin zone is, of course, equivalent to a smaller vector inside the first zone.

We will, however, have to refer to these other vectors in certain situations and it is useful to introduce a terminology for describing them. Suppose we wish, for example, to discuss the *second-smallest* \vec{k} vector for a particular electronic state, i.e., the \vec{k} vector that is smaller than all but one of the vectors in the set of equivalent \vec{k} vectors for this state. Where is this vector located in reciprocal space? In Figure 18.23 below we have added several more bisectors to the Figure 18.22 that we used to describe the first zone. These extra bisectors also enclose



Figure 18.23: Construction of higher zones

various regions of \vec{k} space. Consider the shaded region in Figure 18.23. We reach this region from the origin by crossing one boundary of the first zone. Each \vec{k} vector in this region is *inside* all Brillouin zone boundaries (the bisectors) except one - the one we crossed. Therefore, for each vector in this region there is one and only one smaller \vec{k} vector, namely, $\vec{k} - \vec{G}$, where \vec{G} is the reciprocal lattice translation vector whose bisector we crossed. This region is part of the second Brillouin zone.

The second Brillouin zone is defined as that region of \vec{k} space containing each wave vector that is smaller than all but one of the vectors equivalent to it. Looking at Figure 8.23, there are four parts of the second zone (labelled by II in Figure 18.23). Crossing one more boundary - one of the boundaries of region II - we enter a region of \vec{k} space where each \vec{k} vector is smaller than all but two equivalent \vec{k} vectors. This region is the third Brillouin zone (regions labelled by III in Figure 18.23). In a similar manner the fourth zone can be identified (labelled by IV in Figure 18.23).

Properties of Brillouin Zones

Central to the construction of the first Brillouin zone was the choice of a point as the *origin*. The selection of the origin point, however, is arbitrary. We could have chosen any point of the reciprocal lattice as the origin and constructed a zone identical to the first Brillouin zone.

Alternatively, we could have generated these other regions by translating the first Brillouin zone for some arbitrary origin by various lattice translation vectors \vec{G} eventually filling all of reciprocal space as shown in Figure 18.24 below. Thus, the first Brillouin zone is the primitive unit cell of \vec{k} space.



Figure 18.24: First Brillouin zone as primitive cell

Another property of Brillouin zones that are higher than the first zone is that, although they consist of several disjoint segments, using an appropriate choice of reciprocal lattice translation vectors \vec{G} , we can translate each segment of any higher zone into the first zone as shown in Figure 18.25 below. When all segments have been translated, they will fully cover the first zone with no overlap, i.e., the area (volume in 3 dimensions) of each zone is identical.

Brillouin Zones in Three Dimensions

We can use the same methods to construct the Brillouin zones for three-dimensional lattices. The main difference is that the perpendicular bisectors of the reciprocal lattice vectors \vec{G} are planes instead of lines. As an example we consider a simple cubic lattice.



Figure 18.25: Translating higher zone to first zone

Brillouin Zones of a Simple Cubic Lattice

The three-dimensional analog of the square lattice is the simple cubic lattice which is described by three mutually orthogonal primitive lattice translation vectors

$$\vec{a} = d\hat{x}$$
 , $\vec{b} = d\hat{y}$, $\vec{c} = d\hat{z}$ (18.57)

The reciprocal lattice of a simple cubic lattice is also simple cubic. The separation distance between reciprocal lattice points is $2\pi/d$. The primitive lattice translation vectors defining the reciprocal lattice are

$$\vec{A} = \frac{2\pi}{d}\hat{x}$$
 , $\vec{B} = \frac{2\pi}{d}\hat{y}$, $\vec{C} = \frac{2\pi}{d}\hat{z}$ (18.58)

To construct the first Brillouin zone, we choose a point of the reciprocal lattice as the origin and draw reciprocal lattice translation vectors to all adjacent points of the lattice.

The perpendicular bisectors (planes) of these vectors defines a volume which is the first Brillouin zone. The bisectors, in this case (see figure below) are six planes perpendicular to the

$$\hat{x}(100)$$
 , $\hat{y}(010)$, $\hat{z}(001)$ (18.59)

axes and intersecting these axes at $\pm \pi/d$. The first zone, as shown in Figure 18.26 below, forms a cube. The second Brillouin zone of the simple cubic lattice is a little more difficult to visualize because it involves more intersecting planes. It is defined by these boundaries



Figure 18.26: First Brillouin zone of Simple Cubic Lattice

- 1. the 6 planes that enclose the first Brillouin zone
- 2. the 12 planes that are orthogonal to the (110) axes and intersect these axes at $\pm \sqrt{2}(\pi/d)$ as shown in the Figure 18.27 below.



Figure 18.27: Second Brillouin zone of Simple Cubic Lattice

Figure 18.28 below show three typical segments of the second Brillouin zone.



Figure 18.28: Parts of the Second Brillouin zone

The second zone is a dodecahedron with a cube(first zone) removed from its center.

Electronic States in a Brillouin Zone

Keep in mind that the significance of each vector in \vec{k} space resides in its effect on the electronic state of the crystal $\psi_{E,\vec{k}}(\vec{r})$. In order to determine an analytic form for this function we must solve the Schrodinger equation for the crystal.

Whatever the form of the wave function, however, we know that it satisfies Bloch's theorem

$$\psi_{E,\vec{k}}(\vec{r} + \vec{T}) = e^{ik \cdot T} \psi_{E,\vec{k}}(\vec{r})$$
(18.60)

Each different \vec{k} vector in the first Brillouin zone corresponds to a different electron state. We now ask the question: How many *distinct* electronic states are represented by wave vectors in the first Brillouin zone?

If the crystal were actually infinite, then there are an infinite number of different wave vectors in the first zone and hence the number of electronic states is also infinite. However, no real crystal is truly infinite. We now see how to take this fact into account. We denote by N the number of primitive unit cells in the crystal. We will now prove that there are exactly N electronic state in the first Brillouin zone, i.e., N distinct \vec{k} vectors in that zone. Since each electronic state can be occupied by at most two electrons, one with spin up and one with spin down, the electronic states in the first zone can be occupied by at most 2N electrons.

We do the proof in one dimension (it can easily be extended to 2– and 3–dimensions). We consider a 1–dimensional crystal of length L with lattice spacing d (so that L = Nd since there are N primitive cells). We associate a basis with each lattice point. We are only interested in bulk properties so we neglect edge effects and assume that L, the length of the crystal, is chosen so that we have *periodic boundary conditions*

$$\psi_{E\,\vec{k}}(0) = \psi_{E\,\vec{k}}(L) \tag{18.61}$$

i.e., the crystal repeats itself forever!

This gives, using Bloch's theorem

$$\psi_{E,\vec{k}}(0) = \psi_{E,\vec{k}}(\vec{L}) = e^{i\vec{k}\cdot\vec{L}}\psi_{E,\vec{k}}(\vec{L})$$
(18.62)

or that

$$e^{i\vec{k}\cdot\vec{L}} = 1 \rightarrow \vec{k}\cdot\vec{L} = kL = kNd = 2\pi n$$
, $n = \text{ integer}$ (18.63)

Thus,

$$k = \frac{2\pi n}{L} = \frac{2\pi}{d} \left(\frac{n}{N}\right) \quad , \quad n = 0, \pm 1, \pm 2, \dots, \pm \frac{N}{2}$$
(18.64)

The reciprocal lattice of this direct lattice is a lattice in \vec{k} space of equally spaced points with separation of adjacent point equal to $2\pi/d$.

The first Brillouin zone extends from $-\pi/d$ to $+\pi/d$, such that

$$k = \pi/d \to n = N/2 \tag{18.65}$$

$$k = -\pi/d \to n = -N/2 \tag{18.66}$$

Thus, for the values of \vec{k} in the first zone, the integer *n* can assume all integral values in the range [-N/2, +N/2] and there are *N* integers in this range.

This result says that there are N electronic states in each Brillouin zone.

All of these ideas form the basis of the detailed discussion of the electronic states and energies in a crystal, which we now begin.

18.3 Free-Electron and Weak-Binding Approximations;1-Dimension

The complexity of the potential energy function for a real crystal makes direct solution of the associated exact Schrodinger equation impossible. We must make

approximations in order to learn something about the energies of the electronic states.

We will use two approximations in these notes.

First, we will use the so-called *free-electron approximation* in which the crystal potential energy function is replaced by a constant. This is a very simple and a very crude approximation. It reflects only the fact that the electron is constrained to move within the crystal.

After learning as much as we can from the free-electron approximation, we reintroduce the periodic nature of the crystal potential energy in the so-called *weak-binding approximation*. In using the second approximation we will only look for qualitative solution. We also start with a simple one dimensional system for simplicity.

We will not attempt to find explicit forms for the electronic wave functions, but instead concentrate on determining the energy eigenvalues. In particular, we shall only attempt a determination of graphs for the energy versus the wave vector and the density of states as a function of the energy. These features will enable us to get a clear picture of what is happening in crystals due to translational symmetry.

18.3.1 The Free-Electron Approximation

The potential energy of an electron in a crystal is a periodic function of *vecr* and has singularities at the nuclear sites. The dominant effect of the potential on the electron is to keep it confined inside the crystal. If this is the case, then we can neglect the periodicity and the singularities in a the free-electron approximation and determine what we might call a zero-order picture of the energy as a function of the wave vector. This picture will then be modified in a weak-binding approximation by reimposing periodicity and the singularities so that the basis structure of the energy versus wave vector curve remains basically unchanged except where the added constraints are dominant. That is the reason for the name weak-binding.

We illustrate this approximation in Figure 18.29 below. The dashed line in the figure represents V(x) in the free-electron approximation. It is just a finite square well in one dimension. It is equivalent to replacing the periodic potential with its average value.



Figure 18.29: Free Electron Approximation

Electronic Wave Functions

In this finite square well approximation, the Schrodinger equation inside the crystal is that of a free particle

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi_E(\vec{r}) = E\psi_E(\vec{r})$$
(18.67)

The solutions are the plane-wave eigenfunctions of the free-particle Hamiltonian

$$\psi_E(\vec{r}) = A e^{i k' \cdot \vec{r}} \tag{18.68}$$

with energy eigenvalues

$$E = \frac{\hbar^2 k'^2}{2m_e}$$
(18.69)

where \vec{k}' is the wave vector related to the linear momentum of the particle by $\vec{p} = \hbar \vec{k}'$.

12pt] The solution is in the form of a Bloch function

$$\psi_{E,\vec{k}'}(\vec{r}) = e^{ik'\cdot\vec{r}} u_{E,\vec{k}'}(\vec{r}) \to u_{E,\vec{k}'}(\vec{r}) = A$$
(18.70)

At this point, no limit has be imposed on \vec{k}' . It is called an *extended-zone-scheme* wave vector. In this case, \vec{k}' is a redundant label because the E and \vec{k}' are simply related by the (18.69).

As we said earlier, however, we usually choose the wave vector \vec{k} in Bloch's theorem to be the smallest of the set of equivalent wave vectors, which is called a *reduced-zone-scheme* wave vector. This wave vector \vec{k} is related to \vec{k}' by $\vec{k}' - \vec{k} = \vec{G}$, where \vec{G} is a reciprocal lattice translation vector.

In the reduced zone scheme we can also write the wave function as a Bloch wave using

$$\psi_{E,\vec{k}}(\vec{r}) = Ae^{i\vec{G}\cdot\vec{r}}e^{i\vec{k}\cdot\vec{r}} \to u_{E,\vec{k}}(\vec{r}) = Ae^{i\vec{G}\cdot\vec{r}}$$
(18.71)

In the reduced zone scheme, both the energy and \vec{k} labels are required since these two quantities are no longer simply related as in the extended zone scheme.

E(k) for a One-Dimensional Crystal

We will use an E versus k graph to show the relationship between the energies of the electronic states of a crystal and the allowed values of the wave vector \vec{k} . For example, in the 1-dimensional crystal, if we let k take on all values, i.e., $-\infty < k < +\infty$ and plot $E = \hbar^2 k^2 / 2m_e$, we obtain the parabola shown in Figure 18.30 below. On the horizontal axis - the k-axis - we find values of k from every



Figure 18.30: E versus k - Extended Zone Scheme

Brillouin zone of the lattice and corresponding to each k value there is an E value.

The plot of E versus k above is in the *extended zone scheme*, i.e., it contains values of k from all Brillouin zones. The labeled k values correspond to the Brillouin zone boundaries.

Our earlier discussions imply that as far as Bloch's theorem is concerned , the only significant values of k are those in the first Brillouin zone.

As we saw earlier, for a 1-dimensional crystal with N primitive unit cells, the allowed values of k in the first zone are given by

$$k = \frac{2\pi}{d} \left(\frac{m}{N}\right)$$
, $m = 0, \pm 1, \pm 2, \dots, \pm \frac{N}{2}$ (18.72)

Since N is a very large number, in general, the values of k are very closely spaced.

We can restrict our attention to the first Brillouin zone by plotting E versus k in the reduced zone scheme. To do so we translate all \vec{k} vectors in the higher zones on the plot in the extended zone scheme (Figure 18.30 above) into the first zone given by

$$-\frac{\pi}{d} \le k \le +\frac{\pi}{d} \tag{18.73}$$

That means we add the appropriate reciprocal lattice translation vector to \vec{k}' to generate a wave vector in this range,

$$k = k' \pm \frac{2\pi}{d}n'$$
, $n' = \text{integer}$ (18.74)

In Figure 18.31 below we show explicitly how to generate the reduced zone plot.



Figure 18.31: E versus k - Reduced Zone Scheme

The arrows labeled a correspond to n' = 1 and the arrows labeled b correspond to n' = 2.

The final plot in the reduced zone scheme is shown in Figure 18.32 below. We note that in the plot for the reduced zone scheme an infinite number of energies correspond to each value of k in the first zone. There is an electronic wave function corresponding to each energy.

For each k, we can specify a particular wave function by giving the energy, i.e., $\psi_{E,k}$, or we can introduce a new quantum number to distinguish different electronic states with the same value of k. This new quantum number, n, is shown in Figure 18.32 above. We say that each of the ranges of energy corresponding to k in the first Brillouin zone is a *band* and n labels the bands and is called the *band index*. We write $\psi_{n,k}(x)$. Figure 18.32 above shows the first four bands and part of the fifth band of the 1-dimensional crystal.

The wave function for an electron in this crystal with energy $E \leq \hbar^2 \pi^2/2m_e d^2$



Figure 18.32: E versus k - Final Plot in Reduced Zone Scheme

is

$$\psi_{1,k}(x) = Ae^{ikx}$$
, $A^2L = \int_0^L \psi *_{1,k}(x)\psi_{1,k}(x)dx = 1 \rightarrow A = 1/\sqrt{L}$ (18.75)

For an energy in the second band, we have $\psi_{2,k}(x) = Ae^{ik'x}$ where

$$k' = k + \frac{2\pi}{d}$$
 , $k < 0$, $k' = k - \frac{2\pi}{d}$, $k > 0$ (18.76)

and so on for higher bands.

Summarizing the results we have found in this free-electron approximation:

- 1. We can represent the energy eigenvalues of the electron in a 1-dimensional crystal in two ways, namely, the extended-zone (wave vectors take on all values) and the reduced-zone (wave vectors in first Brillouin zone) schemes.
- 2. We defined bands, each representing N values of k and corresponds to states that can be occupied by at most 2N electrons.
- 3. The bands are connected at the Brillouin zone boundaries.

The Density of States in the Free-Electron Approximation

We define wkdk = number of states with wave vectors between k and k + dk. As we have seen, there are two states for each wave vector and the wave vectors

are uniformly spaced along the k-axis since

$$k = \frac{2\pi}{d} \left(\frac{m}{N}\right)$$
, $m = 0, \pm 1, \pm 2, \dots, \pm \frac{N}{2}$ (18.77)

This says that w(k) is a constant (neglecting the discreteness of k). Since there are 2N states in the first Brillouin zone, where $\Delta k = 2\pi/d$, we have

$$w(k)\Delta k = w(k)\frac{2\pi}{d} = 2N \rightarrow w(k) = \frac{Nd}{\pi} = \frac{L}{\pi}$$
, $L = \text{ length of crystal}$ (18.78)

A more interesting physical quantity is D(E), the density of states as a function of the energy. We define

$$D(E)dE$$
 = number of states with energy between E and $E + dE$ (18.79)

For each interval dE we can find a corresponding interval in k space dk. Then D(E) and w(k) are related by

$$D(E)dE = 2w(k)dk$$
 , $k > 0$ (18.80)

where the factor of 2 arises because each value of E corresponds to two values of k - one positive and the other negative. We then have

$$D(E) = \frac{2w(k)}{\frac{dE}{dk}} \tag{18.81}$$

In the free-electron approximation, $E = \hbar^2 k^2 / 2m_e$ so that

$$\frac{dE}{dk} = \frac{\hbar^2}{m_e}k\tag{18.82}$$

and the density of states in the free-electron approximation is

$$D(E) = \frac{L\sqrt{2m_e}}{\pi\hbar} E^{-1/2}$$
(18.83)

Figure 18.33 above shows that the density of states is largest at small energies and falls off as E increases. Note that we are not restricting k to the first Brillouin zone in this discussion, although we are taking it to be positive.

The Fermi Energy

Each band in a crystal can be occupied by as many as 2N electrons. Electrons have half-integral spin and are fermions. In the orbital approximation the occupation of electronic states by these electrons is governed by Fermi-Dirac statistics. We thus define f(E) = probability that an electronic state with energy E will be occupied by an electron(the distribution function). We then have

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$
(18.84)



Figure 18.33: Density of states D(E)



Figure 18.34: Fermi-Dirac Distribution Function

where $k_B = 1.380622 \times 10^{-16} erg/^{\circ} K$ = Boltzmann's constant, T is the temperature, and μ is a constant that is independent of T. The distribution function is shown in Figure 18.34 below.

The dashed line corresponds to T = 0 and the solid line corresponds to $k_B T \ll \mu$.

The product D(E)f(E) is equal to the density of occupied electronic states. As can be seen from Figure 18.34 above, at T = 0 we find that there is an energy E_F such that all states with $E < E_F$ are occupied but no states with $E > E_F$ are occupied. E_F is called the *Fermi energy*. At T = 0 the Fermi energy is the maximum energy of the electrons in the crystal and is equal to the constant μ in the distribution function. We can define a wave vector k_F corresponding to the Fermi energy (the Fermi wave vector).

To obtain an expression for k_F we introduce a new quantity η , defined to be the number of electrons per primitive unit cell in the crystal. The total number of electrons in the crystal is given by $N\eta$. At T = 0, the total number of occupied states is given by

$$2\int_{0}^{k_{F}}w(k)dk = N\eta \qquad (18.85)$$

Using

$$w(k) = \frac{Nd}{\pi} \tag{18.86}$$
we get

$$k_F = \frac{\pi}{2d}\eta\tag{18.87}$$

The corresponding Fermi energy in the free-electron approximation is then

$$E_F = \frac{\hbar^2}{2m_e} k_F^2 = \frac{\hbar^2}{32m_e d^2} \eta^2$$
(18.88)

In the figures below we show the location of the Fermi energy on plots of E versus k in the extended and reduced zone schemes and on a plot of D(E) versus E. We also show the Fermi energies (and Fermi wave vectors) for various values of η .



Figure 18.35: Fermi Energy in Extended Zone Scheme - Various η values

The arrows label the Fermi energies and Fermi wave vectors in the figures above and below.

Notice that as the number of electrons per primitive unit cell increases, the Fermi energy, and hence the number of occupied states, increases. The Fermi energy enables us to describe the occupation of electronic states in the crystal (at T = 0), and in the 1-dimensional free-electron approximation it can be calculated knowing only the repeat distance d and the number of electrons per primitive unit cell η .

The shaded region shows the occupied states for a crystal with $\eta = 2$.



Figure 18.36: Fermi Energy in Reduced Zone Scheme - Various η values



Figure 18.37: Occupied states on D(E) plot - Various η values

18.4 Introduction to the Weak-Binding Approximation

We must now introduce the periodicity of the crystal potential energy. We write

$$\hat{H} = \hat{T} + \hat{V}(x)$$
 (18.89)

where $\hat{V}(x)$ has the periodicity of the crystal. We assume that the electron interactions due to the potential energy is weak and they still move easily within the crystal, although they are now influenced by the periodic potential. This is the so-called *weak-binding approximation*. We still cannot solve the exact Schrodinger equation. How can we introduce the weak periodic potential and also use all the results of the free-electron approximation.

One possible approach is to use *perturbation theory*, where the free-electron approximation is used as the zeroth-order solution and $\hat{V}(x)$ as the perturbation Hamiltonian. For example, using

$$\psi_{E,k}^{(0)}(x) = \frac{1}{\sqrt{L}} e^{ikx} \tag{18.90}$$

as the zeroth-order wave functions, the first-order perturbed wave function can be written as

$$\psi_{E,k}(x) = \psi_{E,k}^{(0)}(x) + \sum_{k' \neq k} \frac{\langle k' | \hat{V} | k \rangle}{E^{(0)}(k) - E^{(0)}(k')} \psi_{E,k'}^{(0)}(x)$$
$$= \frac{1}{\sqrt{L}} e^{ikx} + \sum_{k' \neq k} \frac{V_{k'k}}{(\hbar^2 k^2 / 2m_e) - (\hbar^2 k'^2 / 2m_e)} \left(\frac{1}{\sqrt{L}} e^{ik'x}\right)$$
(18.91)

where

$$V_{k'k} = \langle k' | \hat{V} | k \rangle = \frac{1}{L} \int_{-L/2}^{+L/2} e^{i(k-k')x} V(x) dx$$
(18.92)

This expression represents a mixing of the functions $e^{ik'x}$ with the zeroth-order function e^{ikx} to form the first-order approximate wave function.

If perturbation theory is valid in this case, then the above result is a good approximation to the electronic wave function.

Let us assume that this approximation is valid and investigate the summation term. The summation is over all allowed wave vectors so it represents a large number of terms. We ask the question - are there any terms where $V_{k'k} = 0$? If so, then these functions do not mix with

$$\psi_{E,k}^{(0)}(x) = \frac{1}{\sqrt{L}}e^{ikx}$$

We can answer this question by applying the translation operator \hat{T}_{op} on the integrand of $V_{k'k}$. This leaves $V_{k'k}$ unchanged since it simply corresponds to redefining the zero of the dummy variable of integration, x, and we may consider the integral to extend from $-\infty$ to $+\infty$ if $nd \ll L$. For a 1-dimensional crystal, any lattice translation vector can be written as nd so we have

$$V_{k'k} = \frac{1}{L} \int_{-L/2}^{+L/2} \hat{T}_{op} e^{i(k-k')x} V(x) dx = \frac{1}{L} \int_{-L/2}^{+L/2} e^{i(k-k')(x+nd)} V(x+nd) dx \quad (18.93)$$

Since V(x) is invariant under translation, we have

$$V_{k'k} = \frac{1}{L} \int_{-L/2}^{+L/2} e^{i(k-k')(x+nd)} V(x) dx = e^{i(k-k')nd} V_{k'k}$$
(18.94)

This result says that the matrix element $V_{k'k} = 0$ unless

$$e^{i(k-k')nd} = 1 \tag{18.95}$$

This is the definition of a reciprocal lattice translation vector. Therefore, we have shown that the only states that mix with $\psi_{E,k}^{(0)}(x)$ in a first-order perturbation calculation are states with wave vectors k' differing from k by reciprocal lattice vectors. All other functions $e^{ik'x}$ can be discarded from the summation, which can then be written

$$\psi_{E,k}(x) = \frac{1}{\sqrt{L}} e^{ikx} + \sum_{G \neq 0} \frac{V_G}{(\hbar^2 k^2 / 2m_e) - (\hbar^2 (k - G)^2 / 2m_e)} \left(\frac{1}{\sqrt{L}} e^{i(k - G)x}\right)$$
(18.96)

where

$$V_G = \frac{1}{L} \int_{-L/2}^{+L/2} e^{iGx} V(x) dx$$
 (18.97)

Since both V(x) and e^{iGx} are periodic, V_G can be written as the integral over one primitive unit cell

$$V_G = \frac{1}{L} N \int_{-d/2}^{+d/2} e^{iGx} V(x) dx = \frac{1}{d} \int_{-d/2}^{+d/2} e^{iGx} V(x) dx$$
(18.98)

This important result - that the only free-electron wave functions that mix with $\psi_{E,k}^{(0)}(x)$ are those wave vectors k' satisfying k'-k = G for some reciprocal lattice vector G - can be shown to hold in any order of perturbation theory. It is true, in fact, even if perturbation theory breaks down!

The energy to second order can be written as

$$E_k \approx \frac{\hbar^2 k^2}{2m_e} + \sum_{G \neq 0} \frac{|V_G|^2}{(\hbar^2 k^2 / 2m_e) - (\hbar^2 (k - G)^2 / 2m_e)}$$
(18.99)

where k is the wave vector in the extended zone scheme and hence $\hbar^2 k^2/2m_e$ is the energy in zeroth order.

Validity of Perturbation Theory

This analysis depends on the question: Is perturbation theory valid for this problem?

The first-order expression for the wave function is a good approximation to the true electronic wave function provided that none of the states in the summation over G mixes strongly with $\psi_{E,k}^{(0)}(x)$, i.e., provided that

$$\left|\frac{V_G}{(\hbar^2 k^2/2m_e) - (\hbar^2 (k-G)^2/2m_e)}\right| << 1$$
(18.100)

for all $G \neq 0$. If there are states that *mix strongly*, i.e., for which the above inequality is violated, then these states cannot be handled by perturbation theory. We can rewrite the inequality as

$$|V_G| \ll \frac{\hbar^2}{2m_e} |G(2k - G)| \tag{18.101}$$

Since this inequality is violated for any state with $k \approx G/2$ there exist states for which we cannot use perturbation theory (if $V_G \neq 0$). So, as long as V_G is small enough (V(x) is weak enough), there exist some states, i.e., those for which k is not nearly equal to any G/2, for which the perturbation expansion can be used. For these states the above expressions for the first-order wave function and the second-order energy are valid and show that the wave functions and energies differ from their zeroth-order counterparts, although not very much.

In the weak-binding approximation, we assume that the energies of these states is essentially the same as in the free-electron approximation.

On the other hand, for states with k = G/2, perturbation theory cannot be used since the function $e^{i(k-G)x}$ mixes strongly with e^{ikx} . We must treat these states some other way.

It is precisely these cases for which the energy will differ most from the freeelectron energy in the dependence of E on k when we move from the free-electron approximation to the weak-binding approximation.

Strongly Mixed States

Let us look back at the free-electron E versus k plots we developed earlier and locate the states that are strongly mixed. We have found that states with wave vector near k = G/2 will strongly mix with states with wave vector $k' = k - G \approx -G/2$, i.e., the strongly mixed states are those with wave vectors *near opposite Brillouin zone boundaries*. The plots below show (in both the extended zone scheme and the reduced zone scheme) the states that are strongly mixed.

The strongly mixed states are connected by an arrow (see Figure 18.38 and 18.39) and numbered for convenience(triangles indicate the state energies). Because of the restriction k' - k = G, there are at most two electronic states that are close to one another in energy and strongly mixed.



Figure 18.38: Strongly mixed states in Extended Zone Scheme



Figure 18.39: Strongly mixed states in Reduced Zone Scheme

The strongly mixed states are

$$1 \leftrightarrow 2 \quad , \quad 3 \leftrightarrow 4 \quad , \quad 5 \leftrightarrow 6 \tag{18.102}$$

Notice that states 1 and 6 are not strongly mixed even though their wave vectors are near zone boundaries and related by a reciprocal lattice translation vector. These states are widely separated in energy, so the denominator in the perturbation expansion term corresponding to these two states is large, and the states are weakly mixed.

Calculation of the Energy Shifts

We now do a simple calculation to show how the energies of the strongly mixed states are affected by the periodic potential energy. We start with the Schrodinger equation

$$(\hat{H} - E)\psi_E(x) = 0$$
 , $\hat{H} = \hat{T} + \hat{V}(x)$ (18.103)

We are interested in an energy corresponding to two strongly mixed states with wave vectors

$$k \approx G/2 \text{ and } k' = k - G$$
 (18.104)

In this case, we can expand $\psi_E(x)$ in the complete set of free-particle states, summing only over equivalent wave vectors, and keep only the terms with large expansion coefficients for the energy of interest

$$\psi_E(x) \approx a \frac{1}{\sqrt{L}} e^{ikx} + b \frac{1}{\sqrt{L}} e^{ik'x}$$
(18.105)

Note that the two free-particle states (see the reduced zone energy plot above) kept in this expansion are nearly degenerate.

We solve this problem by substituting the two state expansion for the wave function into the Schrodinger equation

$$(\hat{H} - E)\psi_E(x)dx = 0 = (\hat{H} - E)(a|k\rangle + b|k'\rangle)$$
(18.106)

$$\langle k | (\hat{H} - E) (a | k \rangle + b | k' \rangle) = 0 = a (\hat{H}_{kk} - E) + b H_{kk'}$$
(18.107)

$$\langle k'|(\hat{H}-E)(a|k\rangle + b|k'\rangle) = 0 = a\hat{H}_{k'k} + b(H_{k'k'} - E)$$
 (18.108)

These two homogeneous equation have a nontrivial solution only if

$$\begin{vmatrix} \hat{H}_{kk} - E & H_{kk'} \\ \hat{H}_{k'k} & \hat{H}_{k'k'} - E \end{vmatrix} = 0$$
(18.109)

where

$$\hat{H}_{kk} = \langle k | \hat{H} | k \rangle$$

$$= \frac{1}{L} \int_{-L/2}^{L/2} e^{-ikx} \left(\frac{\hbar^2}{2m_e} \frac{d^2}{dx^2} + V(x) \right) e^{ikx} dx = \frac{\hbar^2 k^2}{2m_e}$$
(18.110)

$$\hat{H}_{k'k'} = \langle k' | \hat{H} | k' \rangle$$

$$= \frac{1}{L} \int_{-L/2}^{L/2} e^{-ik'x} \left(\frac{\hbar^2}{2m_e} \frac{d^2}{dx^2} + V(x) \right) e^{ik'x} dx = \frac{\hbar^2 k'^2}{2m_e}$$
(18.111)

$$\hat{H}_{kk'} = \langle k | \hat{H} | k' \rangle = \frac{1}{L} \int_{-L/2}^{L/2} e^{-ikx} \left(\frac{\hbar^2}{2m_e} \frac{d^2}{dx^2} + V(x) \right) e^{ik'x} dx$$
$$= \frac{1}{L} \int_{-L/2}^{L/2} e^{i(k'-k)x} V(x) dx = V_{-G} = V_G^*$$
(18.112)

$$\hat{H}_{k'k} = \langle k' | \hat{H} | k \rangle = \frac{1}{L} \int_{-L/2}^{L/2} e^{-ikx} \left(\frac{\hbar^2}{2m_e} \frac{d^2}{dx^2} + V(x) \right) e^{ikx} dx$$
$$= \frac{1}{L} \int_{-L/2}^{L/2} e^{i(k-k')x} V(x) dx = V_G$$
(18.113)

Solving for the energy eigenvalues we get

$$(\hat{H}_{kk} - E)(\hat{H}_{k'k'} - E) - H_{kk'}\hat{H}_{k'k} = 0$$
(18.114)

$$E^{2} - (\hat{H}_{kk} + \hat{H}_{k'k'})E - H_{kk'}\hat{H}_{k'k} = 0$$
(18.115)

 \mathbf{or}

$$E = \frac{1}{2} \left[\frac{\hbar^2 k^2}{2m_e} + \frac{\hbar^2 k'^2}{2m_e} \right] \pm \frac{1}{2} \sqrt{\left[\frac{\hbar^2 k^2}{2m_e} - \frac{\hbar^2 k'^2}{2m_e} \right]^2 + 4 \left| V_G \right|^2}$$
(18.116)

We are especially interested in the behavior of these energies at or near a Brillouin zone boundary. At a zone boundary, we have

$$|k| = |k'| = G/2 \tag{18.117}$$

and thus

$$E = \frac{\hbar^2 k^2}{2m_e} \pm |V_G|$$
 (18.118)

This result shows that the energies of the two strongly mixed states at a zone boundary are split about their average energy

$$\frac{\hbar^2 k^2}{2m_e} \tag{18.119}$$

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by an energy separation of $2|V_G|$ which is called a *band gap*. As we shall see shortly, it separates two nearly free-electron bands.

What happens near a zone boundary?

There we have $k \approx G/2$ and $k' \approx -G/2$. If we introduce a new variable κ defined by

$$\kappa = \frac{1}{2}G - k \tag{18.120}$$

we can write

$$E = \frac{\hbar^2}{2m_e} \left(\frac{G}{2}\right)^2 + \frac{\hbar^2 \kappa^2}{2m_e} \pm \frac{1}{2} \sqrt{\left[\frac{\hbar^2 G \kappa}{2m_e}\right]^2 + 4\left|V_G\right|^2}$$
(18.121)

This equation shows that as we move away from a zone boundary, and κ increases, the splitting between the two states with wave vectors k and k' increases. In addition, the average energy of the two states increases.

As we get further away from the zone boundary, we eventually leave the *region* of strongly mixed states.

Once far enough from the boundary so that perturbation theory is valid and can be used to calculate the energy shift, we know that the energies of the electronic states in the weak-binding approximation are nearly the same as the corresponding energies in the free-electron approximation.

If we are only interested in the qualitative (or semiquantitative) behavior of E versus k, we can simply use the free-electron energies far from the boundaries.

Figures 18.40 and 18.41 below show the effect of the periodic potential energy on the first two bands of the free-electron E versus k plot of the one-dimensional crystal in the reduced and extended zone schemes. The dashed lines are the free-electron result.



Figure 18.40: Band Gaps in Reduced Zone Scheme

We can see from the figure that in the weak-binding approximation the energy



Figure 18.41: Band Gaps in Extended Zone Scheme

splitting calculated using the results above, leads to a gap between the first and second bands. The magnitude of the gap, $2|V_G|$ is dependent on the size of the matrix element V_G . This means that the magnitude of the gap between bands 2 and 3 will differ from that of the gap between 1 and 2 and so on.

Bands and band gaps for the first three bands are shown in both the extended and reduced zone schemes in Figures 18.42 and 18.43 below. The dashed lines are the free-electron result.



Figure 18.42: Band Gaps in Reduced Zone Scheme



Figure 18.43: Band Gaps in Extended Zone Scheme

Qualitative Explanation of Band Gaps

Consider the approximate wave function

$$\psi_E(x) \approx a \frac{1}{\sqrt{L}} e^{ikx} + b \frac{1}{\sqrt{L}} e^{ik'x}$$
(18.122)

At the first Brillouin zone boundary, we have

$$|k'| = |k| = \frac{\pi}{d} \tag{18.123}$$

so that the two free-electron wave functions that mix are *degenerate* and are given by

$$\psi_{E,\pm\pi/d}^{(0)}(x) = \frac{1}{\sqrt{L}} e^{\pm i\pi x/d}$$
(18.124)

where the zero superscript reminds us that these are free-electron approximations to the wave function. The two weak-binding wave functions $\psi_E(x)$ at the zone boundary, where $|a| = |b| = 1/\sqrt{2}$ from the solution of the eigenvalue equation can be written as normalized standing-wave eigenfunctions

$$\psi_{E,c}(x) = \frac{1}{\sqrt{2}} \left(\psi_{E,+\pi/d}^{(0)}(x) + \psi_{E,-\pi/d}^{(0)}(x) \right) = \sqrt{\frac{2}{L}} \cos\left(\frac{\pi}{d}x\right)$$
(18.125)

$$\psi_{E,s}(x) = \frac{1}{\sqrt{2}} \left(\psi_{E,+\pi/d}^{(0)}(x) - \psi_{E,-\pi/d}^{(0)}(x) \right) = \sqrt{\frac{2}{L}} \sin s \left(\frac{\pi}{d} x \right)$$
(18.126)

The probability densities $|\psi_{E,c}(x)|^2$ and $|\psi_{E,s}(x)|^2$ for wave vectors at the first Brillouin zone boundary in the case of one atom per primitive unit cell (with the origin at one of the atoms) is shown in Figure 18.44 below.



Figure 18.44: Probability Densities

We see that $\psi_{E,c}(x)$ has a maximum of probability density near each singularity

of the strongly attractive potential energy of the crystal. On the other hand, $\psi_{E,s}(x)$ has a minimum of probability density near each singularity. Consequently, we expect to see a splitting between the energies for these two wave functions. This splitting is just the band gap $2|V_G|$.

Density of States in the Weak-Binding Approximation

How do we modify D(E) in the weak-binding approximation? Our original derivation of w(K) is not dependent on the approximation V(x) = constant. Thus, that derivation is also valid in the weak-binding approximation and we still have

$$w(k) = \frac{Nd}{\pi} = \frac{L}{\pi} \tag{18.127}$$

Similarly, the derivation of the Fermi wave vector is only based on

$$2\int_{0}^{k_{F}}w(k)dk = N\eta$$
 (18.128)

and does not use the assumption of free-electron behavior (it does assume a monotonic increase of E with k in the extended zone scheme). So, in the weakbinding approximation, we still have

$$k_F = \frac{\pi}{2d}\eta \tag{18.129}$$

where η is the number of atoms per primitive unit cell. The expression for the Fermi energy cannot be carried over into the weak-binding approximation because we used the fact the the energy E was quadratic in the wave vector kin the derivation.

Metallic and Nonmetallic Behavior

Now we consider a 1-dimensional crystal with one electron per primitive unit cell ($\eta = 1$). The Fermi wave vector is $k_F = \pi/2d$. For this wave vector the Fermi energy is near the middle of the first band (see the earlier figure). For $\eta = 1$, the first band is half-filled. Since the Fermi energy is the maximum energy for the electrons at absolute zero, no states with $E > E_F$ are occupied. This means that there exist empty states infinitesimally close to the energy of the highest occupied state and an infinitesimal increment of energy can excite an electron to one of these empty states (turn on a small electric field). Thus, for infinitesimal electric fields we get infinitesimal currents (extra kinetic energy).

A crystal that exhibits such behavior is called a *metal*.

In contrast, consider a crystal, with two electrons per primitive unit cell. In this case, $k_F = \pi/d$, which corresponds to the edge of the band - the first band is full, i.e., all the electronic states in this band are occupied at absolute zero. Since

the next nearest empty state is separated from the first band by an energy gap of magnitude $2|V_G|$, at least this much energy is required in order to excite an electron into one of the empty states.

A crystal that exhibits such behavior is called an *insulator*.

18.5 The Kronig-Penney Model

18.5.1 Exact Analysis

The Kronig-Penney model of a crystal consists of an infinite series of square wells as shown in Figure 18.45 below. Each well is of width d-s and depth V_0 .



Figure 18.45: Kronig-Penney Potential

Adjacent wells are separated by a distance s, the width of each barrier. The repeat distance for this crystal - the length of the primitive unit cell - is d. The only restrictions we place on the well parameters at this time are

$$s > 0, \ s < d, \ V_0 > 0$$
 (18.130)

We have not imposed either free-electron or weak-binding behavior. This will be an exact solution.

The Eigenvalue Equation

The Kronig-Penney potential energy is a periodic function, which means that we can use Bloch's theorem to connect the wave functions from different regions of the crystal. In one dimension, the second form of Bloch's theorem says

$$\psi_{E,k}(x) = e^{ikx} u_{E,k}(x) \tag{18.131}$$

where $u_{E,k}(x)$ is a periodic function invariant under translation by any lattice translation vector T = nd, i.e.,

$$u_{E,k}(x+nd) = u_{E,k}(x) \tag{18.132}$$

the relationship between E and k is not known yet.

From the graph(Figure 18.45) of the potential function, we see that there are two regions of potential energy:

- 1. ranges of x for which $V = 0 \rightarrow nd \le x \le nd + (d s)$
- 2. ranges of x for which $V = V_0 \rightarrow nd + (d-s) \leq x \leq (n+1)d$

where $n = 0, \pm 1, \pm 2, \dots$. The form of the wave function is different in these two regions.

In the region $0 \le x \le (d - s)$ the potential energy is zero and the electronic Schrodinger equation is

$$\frac{d^2\psi_{E,k}(x)}{dx^2} + \frac{2m_e}{\hbar^2}E\psi_{E,k}(x) = 0$$
(18.133)

with solutions

$$\psi_{E,k}(x) = Ae^{i\alpha x} + Be^{-i\alpha x}$$
, $\alpha = \frac{1}{\hbar}\sqrt{2m_e E}$ (18.134)

The form of $u_{E,k}(x)$ is then

$$u_{E,k}(x) = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x}$$
(18.135)

Using the same sort of arguments for the region $(d-s) \le x \le d$ where $V = V_0$ we have the electronic Schrödinger equation

$$\frac{d^2\psi_{E,k}(x)}{dx^2} - \frac{2m_e}{\hbar^2}(V_0 - E)\psi_{E,k}(x) = 0$$
(18.136)

with solutions

$$\psi_{E,k}(x) = Ce^{\beta x} + De^{-\beta x} , \quad \beta = \frac{1}{\hbar}\sqrt{2m_e(V_0 - E)}$$
 (18.137)

The form of $u_{E,k}(x)$ is then

$$u_{E,k}(x) = Ce^{(\beta - ik)x} + De^{-(\beta + ik)x}$$
(18.138)

There are four unknowns in these solutions A, B, C and D, but there are also four connecting equations - two for the periodicity conditions and two for the continuity of u and du/dx.

The periodicity conditions give

$$u(0) = u(d) \tag{18.139}$$

$$A + B = e^{-ikd} (Ce^{\beta d} + De^{-\beta d})$$
(18.140)

$$\frac{du}{dx}\Big|_{0} = \frac{du}{dx}\Big|_{d} \tag{18.141}$$

$$i\alpha(A-B) = \beta e^{-ikd} (Ce^{\beta d} - De^{-\beta d})$$
(18.142)

The continuity conditions give

$$\lim_{\varepsilon \to 0} u(d - s + \varepsilon) = \lim_{\varepsilon \to 0} u(d - s - \varepsilon)$$
(18.143)

$$Ae^{i\alpha(d-s)} + Be^{-i\alpha(d-s)} = Ce^{\beta(d-s)} + De^{-\beta(d-s)}$$
(18.144)
, du (18.144)

$$\lim_{\varepsilon \to 0} \left. \frac{du}{dx} \right|_{d-s+\varepsilon} = \lim_{\varepsilon \to 0} \left. \frac{du}{dx} \right|_{d-s-\varepsilon}$$
(18.145)

$$i\alpha(Ae^{i\alpha(d-s)} - Be^{-i\alpha(d-s)}) = \beta(Ce^{\beta(d-s)} - De^{-\beta(d-s)})$$
(18.146)

These four equations have nontrivial solutions only if the determinant of the matrix of the coefficients of A, B, C and D vanishes

Some algebra gives

$$\cos kd = \cos \alpha (d-s) \cosh \beta s + \frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin \alpha (d-s) \sinh \beta s \qquad (18.148)$$

This is a transcendental equation relating the electronic energy E to the quantum number k in the Kronig-Penney model.

Limiting Cases

1. In the limit $V_0 \rightarrow 0$, the particle will be confined to one of the square wells in the model crystal. In this case the energy eigenvalue equation becomes

$$\frac{\cos kd}{\cosh \beta s} = \cos \alpha (d-s) + \frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin \alpha (d-s) \tanh \beta s$$

$$0 = \cos \alpha (d-s) + \frac{\beta}{2\alpha} \sin \alpha (d-s)$$

$$\sin \alpha (d-s) = 0 \rightarrow \alpha (d-s) = n\pi$$

$$\alpha^2 = \frac{n^2 \pi^2}{(d-s)^2} = \frac{2m_e E}{\hbar^2}$$

$$E = \frac{n^2 \pi^2 \hbar^2}{2m_e (d-s)^2}$$
(18.149)

which is the familiar result for a *particle in an infinite box*.

2. Now we keep V_0 finite, fix the width of each well, and let the well separation $s \to \infty$. In this case, wells will be completely isolated from one another and we expect the eigenvalue equation to reduce to the equation for a

particle in a single finite square well. We find

$$0 = \cos \alpha (d - s) + \frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin \alpha (d - s)$$
$$\cot \alpha (d - s) = \frac{\alpha^2 - \beta^2}{2\alpha\beta}$$
(18.150)

which is the standard transcendental equation of the finite square well.

3. Let us remove the periodicity of V(x). There are three ways to do this

$$V_0 \to 0 \text{ or } s \to 0 \text{ or } s \to d$$
 (18.151)

In each case, we get

$$E = \frac{\hbar^2 k^2}{2m_e} \tag{18.152}$$

which is the expected result for a free particle.

Confident that we have arrived at a sensible eigenvalue equation we now look at solutions of the exact equation.

Solutions of the Eigenvalue Equation

A form of the eigenvalue equation that is particularly easy to work with is obtained by considering cases where

$$V_0 \to \infty$$
, $s \to 0$ such that $V_0 s$ remains constant (18.153)

In this case we have

$$\cos kd = \cos \alpha d + \frac{\beta}{2\alpha} \sin \alpha d \sinh \beta s \tag{18.154}$$

$$\cos kd = \cos \alpha d + \frac{\frac{1}{\hbar}\sqrt{2m_e V_0}}{2\alpha} \sin \alpha d \sinh \frac{1}{\hbar}\sqrt{2m_e V_0}s \tag{18.155}$$

$$\cos kd = \cos \alpha d + \frac{\frac{1}{h}\sqrt{2m_eV_0}}{2\alpha} \sin \alpha d\frac{1}{h}\sqrt{2m_eV_0}s \tag{18.156}$$

$$\cos kd = \cos \alpha d + \frac{m_e V_0 sd}{\hbar^2} \frac{\sin \alpha d}{\alpha d}$$
(18.157)

If we choose

$$\frac{m_e V_0 s d}{\hbar^2} = 1 \tag{18.158}$$

we have

$$\cos kd = \cos \alpha d + \frac{\sin \alpha d}{\alpha d} \tag{18.159}$$

This result clearly shows the band structure, that is, since the value of the left hand side of this equation is between 1 and -1, solutions only exist for energies

E such that the magnitude of the right hand side is ≤ 1 .

Energies violating this condition do not correspond to possible states of the particle.

In Figure 18.46 below we plot the right hand side versus αd for $\alpha d \leq 3\pi$.



Figure 18.46: Kronig-Penney Model - Transcendental Plot

We find that the lowest allowed energy of the particle in this Kronig-Penny crystal is

$$E = 0.174 \frac{\pi^2 \hbar^2}{2m_e d^2} \tag{18.160}$$

Looking at the regions lying between +1 and -1 we see the structure of energy bands and band gaps clearly revealed. In particular, the particle can have any

energy in the following ranges

| $0.174 \leq E \leq 1$ | $\rightarrow band$ | 1 |
|-----------------------|--------------------|---|
| $1.370 \leq E \leq 4$ | $\rightarrow band$ | 2 |
| $4.490 \le E \le 9$ | $\rightarrow band$ | 3 |

States of the system exist for any energy in one of these bands. No solution exist if

| $1 \le E \le 1.37$ | $\rightarrow gap$ | 1 |
|--------------------|-------------------|----------|
| $4 \le E \le 4.49$ | $\rightarrow gap$ | 2 |

These results are very different from those obtained by solution of the Schrodinger equation for an atom or molecule. Instead of discrete bound levels, we find continuous bands of allowed energies and intervening gaps of forbidden energies.

A plot of E versus k can be made from the eigenvalue equation. An example is shown in Figure 18.47 below.



Figure 18.47: Energy Bands and Gaps in the Kronig-Penney Model

The dashed line shows the free-electron approximation, i.e., treating the Kronig-Penney model as a giant square well.

Weak-Binding Limit

In this limit we let the well separation s get small. In particular, we assume that s is sufficiently small that the barriers can be treated as a small perturbation on a constant potential energy. In this way, we can approach the weak-binding limit through the exact energies. If s is small we assume that

$$\alpha s \ll 1 \text{ and } \beta s \ll 1 \tag{18.161}$$

In this case, we can write the electronic energy as

$$E = E_0 + \varepsilon = \frac{\hbar^2 k^2}{2m_e} + \varepsilon \tag{18.162}$$

We want to expand the exact eigenvalue equation in the small parameter ε . We write

$$\alpha = \alpha_0 + \alpha_1 = \frac{1}{\hbar} \sqrt{2m_e E_0} + \alpha_1 = \frac{1}{\hbar} \sqrt{2m_e E}$$
(18.163)

$$\beta = \beta_0 + \beta_1 = \frac{1}{\hbar} \sqrt{2m_e(V_0 - E_0)} + \beta_1 = \frac{1}{\hbar} \sqrt{2m_e(V_0 - E)}$$
(18.164)

We then have

$$\alpha_{1} = \frac{1}{\hbar} \sqrt{2m_{e}(E_{0} + \varepsilon)} - \frac{1}{\hbar} \sqrt{2m_{e}E_{0}} = \frac{1}{\hbar} \sqrt{2m_{e}E_{0}} \left((1 + \varepsilon/E_{0}) - 1 \right)$$
$$= \frac{1}{\hbar} \sqrt{2m_{e}E_{0}} \left((1 + \varepsilon/2E_{0} + \dots) - 1 \right) = \frac{m_{e}\varepsilon}{\hbar^{2}k} - \frac{m_{e}^{2}\varepsilon^{2}}{2\hbar^{4}k^{3}}$$
(18.165)

and

$$\beta_{1} = \frac{1}{\hbar} \sqrt{2m_{e}(V_{0} - E)} - \frac{1}{\hbar} \sqrt{2m_{e}(V_{0} - E_{0})}$$
$$= -\frac{\beta_{0}}{2} \frac{\varepsilon}{V_{0} - E_{0}} - \frac{\beta_{0}}{8} \frac{\varepsilon^{2}}{(V_{0} - E_{0})^{2}}$$
(18.166)

Using trigonometric identities for $\sin(a \pm b)$, $\cos(a \pm b)$ and Taylor series expansions of cos, sin, cosh and sinh function, the eigenvalue equation becomes

$$\cos kd = \cos \alpha d + s \frac{\alpha^2 + \beta^2}{2\alpha} \sin \alpha d \qquad (18.167)$$

We can also write

$$\frac{\alpha^2 + \beta^2}{2\alpha} = \frac{\alpha_0^2 + \beta_0^2}{2\alpha_0} - \frac{\alpha_0^2 + \beta_0^2}{2\alpha_0^2} \alpha_1$$
(18.168)

This only retains terms to order ε , but when multiplied by $s \sin \alpha d$ the second order terms are obtained.

Substitution gives

$$\left(-\frac{1}{2}\alpha_1^2 d^2 + \frac{\alpha_0^2 + \beta_0^2}{2\alpha_0} s\alpha_1 d \right) \cos kd + \left(-\alpha_1 d + \frac{\alpha_0^2 + \beta_0^2}{2\alpha_0} s - \frac{\alpha_0^2 + \beta_0^2}{2\alpha_0^2} \alpha_1 s \right) \sin kd = 0$$
 (18.169)

Using this expression we can solve explicitly for the energy for wave vectors at the Brillouin zone boundaries and determine the band gaps.

In the extended zone scheme the boundaries occur at

$$kd = n\pi$$
 , $n =$ integer (18.170)

For these values of k we have

$$\sin kd = 0$$
 , $\cos kd = (-1)^n$ (18.171)

Therefore, at zone boundaries the second term is zero and the first term gives two conditions for α_1

$$\alpha_1 d = 0 \quad or \quad \alpha_1 d = \frac{\alpha_0^2 + \beta_0^2}{\alpha_0} s$$
 (18.172)

The first choice gives $\varepsilon = 0$ and the second choice gives $\varepsilon = 2V_0 s/d$ and thus we get a band gap of energy $\Delta E = 2V_0 s/d$ at the zone boundary in the weak-binding approximation.

18.6 Free-Electron and Weak-Binding Approximations;2-Dimensions

We will now study two-dimensional crystals, examining the behavior of energy as a function of wave vector and of the density of states as a function of energy.

The study of electron band theory in one dimension was comparatively simple for several reasons. First, there is only one Bravais lattice in one dimension; thus the only difference between various one-dimensional problems arises from such factors as the number of atoms per primitive unit cell, the strength of the potential, and the separation of the lattice points. This situation contrasts strikingly with that in two and three dimensions, where there are 5 and 14 Bravais lattices, respectively, each of which poses its own special problem.

Thus, there is a considerable increase in the complexity of any calculation in band theory as the number of dimensions increases.

18.6.1 The Free-Electron Approximation

Let us consider a two-dimensional crystal in the free-electron approximation, that is, we shall neglect the periodic part of the crystal potential energy V(x, y)and assume that the electrons are free to move about within the confines of the crystal. In this approximation the equation relating the energy of an electronic state to the wave vector is

$$E = \frac{\hbar^2 k^2}{2m_e}$$
(18.173)

where the two-component wave vector can be expressed as

$$\vec{k} = k_x \hat{x} + k_y \hat{y} \tag{18.174}$$

In order to see the basic structure of such a crystal, we must examine plots of E versus k. Since k is a two-component vector, E(k) is a paraboloid of revolution, as shown in Figure 18.48 below in the extended zone scheme.



Figure 18.48: E(k) paraboloid

Eventually we will want to use the reduced zone scheme and identify E versus k graphs so as to incorporate the periodic nature of $V(\vec{r})$. It is clear that each, of these steps is rather difficult if we use the three-dimensional graph in Figure 18.48.

Moreover, even if we could draw the resulting diagrams, their complexity might obscure some of the information they contain.

For this reason, we will now introduce two other ways of representing the energy of the electronic states of a crystal.

${\it E}$ versus Path Distance

The first requires that we pick a path in k space (i.e., a continuous connected set of line segments) and plot the energy as a function of the distance along this

path. We will represent the distance along the path by the integral

$$\int_{c} dk \tag{18.175}$$

For example, suppose that we choose the path shown in Figure 18.49 below.



Figure 18.49: Path in k space

Using the quadratic relation between E and k for the energy in the free-electron approximation, we can sketch E as a function of distance along this path, obtaining the curve shown in Figure 18.50 below (in the extended zone scheme).



Figure 18.50: E versus path in k space

We shall return to this technique frequently.

Constant Energy Contours

An alternate representation of the energy can be obtained by choosing several different values of energy and plotting curves in k space that correspond to these constant values of E. Such curves are called constant energy contours. In the free-electron approximation, where E(k) is quadratic in k, each curve of constant energy is a circle of radius

$$k = \frac{1}{\hbar}\sqrt{2m_eE} \tag{18.176}$$

As E increases, the radius of the circle increases. Thus we obtain a series of concentric circles; several constant energy contours are shown in Figure 18.51 below, where the extended zone scheme is used.



Figure 18.51: Constant energy contours in k space

Notice that $E_1 < E_2 < E_3 < E_4 < E_5$.

Now, in going to the reduced zone scheme, we must specify a particular type of Bravais lattice. Recall from our earlier discussion that there are five Bravais lattices in two dimensions: the oblique lattice, the primitive rectangular lattice, the centered rectangular lattice, the square lattice, and the hexagonal lattice. To illustrate the preparation of graphs of E versus path distance and constant energy contours, we choose the square lattice. Let d denote the spacing of adjacent lattice points in the x or y direction in the square lattice. Then the

The Square Lattice

In order to plot E versus path length for the square lattice, we must first select a path. The choice of path is somewhat arbitrary, but common sense can guide us. Since we want to generate a plot in the reduced zone scheme, where only values of k in the first Brillouin zone are considered, we should choose a path contained in that zone or on one of its boundaries. We would like the path to be as simple as possible, and, ideally, each segment of the path should provide some new information about the behavior of E(k).

The reciprocal of the square lattice is square and possesses fourfold symmetry. A path that passes through all points of *high symmetry* in the first zone but that does not contain segments equivalent to one another under the symmetry operations of the square lattice is shown in Figure 18.52 below.

We will now compute the value of E at points on this path and on equivalent



Figure 18.52: Path in k space through high symmetry points

paths in the surrounding regions of the reciprocal lattice. In Figure 18.53 below, we have translated the first Brillouin zone and the chosen path throughout a portion of the reciprocal lattice.



Figure 18.53: Equivalent paths in k space by translation

The resulting squares are numbered (1) through (9) for purposes of identification. We have also indicated the value of E in the free-electron approximation at several points in k space - specifically, at the corners of each path (units of energy are $\hbar^2 \pi^2 / 2m_e d^2$). A typical point, say the 13 along the right edge in the (9) box has

$$\vec{k} = \frac{3\pi}{d}\hat{x} + \frac{2\pi}{d}\hat{y}$$
(18.177)

so that its energy, in the free-electron approximation, is

$$E = \frac{\hbar^2 k^2}{2m_e} = 13 \frac{\hbar^2 \pi^2}{2m_e d^2}$$
(18.178)

The origin is at the center of the (0) square.

The reason for considering values of k outside the first zone is that we wish to take into account energies greater than $\hbar^2 \pi^2 / 2m_e d^2$, the maximum value of energy that corresponds to points all of which lie within the first zone. Notice that each path in a region other than the first zone is equivalent to the path in the first zone. The wave vectors k' of these equivalent paths will be related to wave vectors in the first zone by some reciprocal lattice translation vector

$$\vec{k}' = \vec{k} + \vec{G}$$
 (18.179)

Several different methods exist to generate data like that shown in the above figure - and hence the resulting free-electron energy bands. The following steps will enable us to obtain the necessary information in a fairly organized way:

(1) Draw all paths with |k'| less than some maximum value corresponding to an upper limit on the energy for which the resulting bands will be *accurate* (we choose $3\pi/d$ for the upper limit on k' in this example).

We will guarantee an accurate sketch of E versus $\int_{c} dk$ only for energies below $\hbar^{2}k_{\max}^{2}/2m_{e}$, where k_{max} is the maximum value of |k'|. Above this energy, we may not have included all the necessary path segments.

(2) Calculate the energy E in reduced units $\hbar^2 \pi^2 / 2m_e d^2$.

$$\frac{E}{\hbar^2 \pi^2 / 2m_e d^2} = \left(\frac{\vec{k}}{\pi/d}\right)^2 = \left(\frac{k_x}{\pi/d}\right)^2 + \left(\frac{k_y}{\pi/d}\right)^2 \tag{18.180}$$

for each *important point* on the path. (In this case, the three corners of the triangular paths are the *important points*, for it is there that the path changes direction and the relationship of E to $\int dk$ is altered.

We now use the data in Figure 18.53 to plot the energy in the reduced zone scheme for each path. These energies are then connected by segments of a parabola. This process yields the desired plot of E versus path distance.

For this example, the plot is shown in Figures 18.54-18.60 below. Notice that

in the free-electron approximation portions of some of the paths are degenerate in energy. Most of this degeneracy will be lifted in the weak-binding approximation(degenerate curves in this figure have more than one number associated with them). We have plotted a sequence of graphs showing each path being added.



Figure 18.54: Step #1



Figure 18.55: Step #2



Figure 18.57: Step #4

(1,0)

(1,1)

 $\frac{d}{\pi}(k_x,k_y)$

1 (0,0)

5

0

(0,0)



Figure 18.59: Step #6



Figure 18.60: Step #7

Above, we have shown the energy versus path distance for the nine paths in the free-electron approximation. The energy is plotted in reduced units. The little numbers beside each path segment correspond to the path indices (1) through (9) of the earlier figure. The arrow indicates the upper energy limit corresponding to $|k'| = 3\pi/d$.

Notice carefully that the figure does not show the energy bands explicitly. However, we can extract them from this sketch.

The curve of E versus path distance that is everywhere lowest in energy corresponds to the first band, the curve that is second lowest in energy corresponds to the second band, and so on.

Thus we need only examine the figure in each region of $(d/\pi)(k_x, k_y) - (0, 0)$ to (1, 0), (1, 0) to (1, 1), and (1, 1) to (0, 0) – and select the first, second.... lowest curves to obtain plots of E versus path distance for the first, second, ... bands. We have extracted the first nine bands in Figure 18.61 below.



Figure 18.61: First 9 Bands

The section of this graph between (0,0) and (1,0) shows the first nine bands in the reduced zone scheme for the free-electron approximation.

We see from the figure that paths 1, 2, and 3 each correspond to a single energy band, a fortuitous consequence of the triangular path chosen.

However, path 4 does not correspond everywhere to the fourth lowest energy. Part of path 5 falls below path 4, and so the fourth energy band is made up of contributions from paths 4 and 5.

In general, all bands higher than the first (lowest) have a complicated structure, with contributions from parts of several paths. (This situation occurs because a general path will cross at least one Brillouin zone boundary and so cannot correspond to a single energy band).

Constant Energy Contours

Consider now the second representation of the E versus k relationship for the square lattice, namely, constant energy contours.

The objective of this method is to display the variation of energy with k for each band in the reduced zone scheme.

We will begin in the extended zone scheme, with several Brillouin zones, and draw constant energy contours. These contours can be translated into the first zone by appropriate reciprocal lattice translation vectors. Such translation of segments of higher zones into the first zone was discussed earlier.

The first four Brillouin zones of the square lattice were shown earlier in Figure 18.23.

In Figure 18.62 below, we have extended this sketch to show the first seven zones and have also drawn contours of constant energy that lie entirely within these zones in the free-electron approximation for the square lattice.



Figure 18.62: First 7 zones with energy contours - square lattice

In Figure 18.63 below we show the portions of these contours that lie in the first zone, together with the free-electron energies (in reduced units) at several points of the first zone. These are constant energy contours for the first band of energy.



Figure 18.63: Energy contours in first band

To obtain contours for the second band, we translate the segments of the second Brillouin zone from the figure above into the first zone, carrying along the appropriate arcs.

The sequence of steps and the resulting reduced zone scheme constant energy contours are shown in Figures 18.64-18.66 below.



Figure 18.64: Energy contours in extended scheme



Figure 18.65: Translating contours to second band regions



Figure 18.66: Energy contours in second band

Similar constructions yield the higher bands.

Notice the behavior of the energy for each band. For example, the second band has a minimum in energy at the center of the edge of the Brillouin zone, As we approach a corner of the zone, the energy increases monotonically to 2; as we go toward the center of the zone, the energy increases to its maximum value of 4.

The Fermi Surface

Earlier we defined an energy E_F called the Fermi energy, with the property that, at absolute zero, states with energies $E > E_F$ are not occupied but states with energies $E < E_F$ are occupied. Corresponding to the Fermi energy is the Fermi wave vector k_F . We saw that both quantities depend on η , the number of electrons per primitive unit cell.

The wave vectors of the occupied states each satisfy $|\vec{k}| < k_F$ (in the extended zone scheme). Therefore we can view the points $\pm k_F$, as defining a one-dimensional *surface* enclosing values of k that correspond to occupied states. Similarly, we can define a Fermi *surface* in two dimensions corresponding to the Fermi energy E_F . In the free-electron approximation this energy corresponds to one of the constant energy circles introduced earlier (in the extended zone scheme). The radius of this circle is k_F , the Fermi wave vector. Again, each state with an energy less than E_F is occupied at absolute zero. The corresponding constant energy contour will lie within the Fermi *surface*. Let us derive expressions for k_F and E_F in the free-electron approximation and then locate the Fermi surfaces for the square lattice. The derivations will be similar to their one-dimensional counterparts we carried out earlier. We denote by q the area in k space of the first Brillouin zone. The number of states *in* this zone is 2N, where N is the number of primitive unit cells in the crystal. Thus $w(\vec{k})$ is equal to 2N/q, a result completely equivalent to our earlier result. The total number of electrons in the crystal is [from earlier]

$$\int_{0}^{k_{F}} w(\vec{k}) d\vec{k} = \pi k_{F}^{2} \frac{2N}{q}$$
(18.181)

But there are ηN electrons in the crystal, so we have

$$\eta N = \pi k_F^2 \frac{2N}{q} \tag{18.182}$$

which implies that the Fermi wave vector is

$$k_F = \sqrt{\frac{q}{2\pi}\eta} \tag{18.183}$$

The Fermi energy in the free-electron approximation is

$$E_F = \frac{\hbar^2 k_F^2}{2m_e} = \frac{\hbar^2}{2m_e} \frac{q}{2\pi} \eta$$
(18.184)

These results apply to any two-dimensional crystal. To illustrate, we will apply them to the square lattice.

The area of the first Brillouin zone of the square lattice is

$$q = \left(\frac{2\pi}{d}\right)^2 \tag{18.185}$$

where d is the lattice separation in coordinate space. Therefore, the Fermi wave vector is _____

$$k_F = \frac{\pi}{d} \sqrt{\frac{2\eta}{\pi}} \tag{18.186}$$

and the Fermi energy is

$$E_F = \frac{\hbar^2}{2m_e} \left(\frac{\pi}{d}\right)^2 \frac{2\eta}{\pi} \tag{18.187}$$

Table 18.4 below shows values of k_F and E_F for $\eta=1\to\eta=6$ for the two-dimensional square lattice.

| η | $k_F(\pi/d)$ | $E_F(\hbar^2\pi^2/2m_ed^2)$ |
|--------|--------------|-----------------------------|
| 1 | 0.798 | 0.637 |
| 2 | 1.128 | 1.273 |
| 3 | 1.384 | 1.910 |
| 4 | 1.596 | 2.546 |
| 5 | 1.784 | 3.183 |
| 6 | 1.954 | 3.820 |

Table 18.4: Two-dimensional square lattices values

The corresponding Fermi surfaces are shown in the extended zone scheme in Figure 18.67 below.



Figure 18.67: Fermi surfaces

The circle with the smallest radius corresponds to $\eta = 1$; the one with the largest radius to $\eta = 6$. In Figure 18.68 below these Fermi surfaces are translated into the first Brillouin zone. The shaded parts correspond to occupied states at absolute zero (wave vectors with energies less than E_F .


Figure 18.68: Fermi surfaces translated to first zone

Let us look at these sketches. For q = 1, the entire Fermi surface lies within the first Brillouin zone. Thus all occupied states have energies within the first band. Notice that there are states with energies in the first band that are not occupied. This fact is also reflected by the E versus path distance graph for the first four bands. This graph is reproduced in Figure 18.69 below, where we show the location of the Fermi energies.



Figure 18.69: First 4 bands with location of Fermi surfaces

For crystals with 2 or 3 electrons per primitive unit cell, we see from (b) in Figure 18.68 and Figure 18.69 above that there are occupied states in the first and second bands; neither of these bands is completely filled. In contrast, the first band is filled for crystals with $\eta \ge 4$.

The Weak-Binding Approximation

We will now improve on the free-electron approximation by introducing the periodicity of the crystal potential energy. We approach this task via the weakbinding approximation discussed earlier, which assumes that the electrons are not too strongly bound to the individual nuclei of the crystal. In particular, we will ignore states that can be treated by time-independent perturbation theory and concentrate on the strongly mixed states.

As earlier, we can determine which states are strongly mixed by examining the matrix elements of the crystal potential energy. As earlier, this matrix element is defined as

$$V_{\vec{k}'\vec{k}} = \langle \vec{k}' | \hat{V} | \vec{k} \rangle = \frac{1}{A} \int d\vec{r} e^{-i\vec{k}'\cdot\vec{r}} V(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$
(18.188)

where

$$\left\langle \vec{r} \mid \vec{k} \right\rangle = \frac{1}{\sqrt{A}} e^{i\vec{k}\cdot\vec{r}} \quad , \quad \left\langle \vec{r} \mid \vec{k}' \right\rangle = \frac{1}{\sqrt{A}} e^{i\vec{k}'\cdot\vec{r}} \tag{18.189}$$

are normalized free-electron wave functions of energy

$$\frac{\hbar^2 k^2}{2m_e} \quad , \quad \frac{\hbar^2 k'^2}{2m_e} \tag{18.190}$$

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respectively, and where $\vec{r} = x\hat{x} + y\hat{y}$ is a vector in the two-dimensional coordinate space of the direct lattice. Recall from earlier that these matrix elements also appear in the calculation of the energy eigenvalues due to mixing of the strongly mixed states.

An analysis identical to the perturbation discussions earlier reveals that the only states that mix at all, strongly or weakly, with $\psi_{E,\vec{k}}^{(0)}(\vec{r})$ are those with wave vectors \vec{k}' that are related to \vec{k} by a reciprocal lattice translation vector $\vec{k} - \vec{k}' = \vec{G}$. If this relation is not satisfied, then $V_{\vec{k}'\vec{k}} = 0$.

We can write the nonzero matrix elements as

$$V_{\vec{G}} = \frac{1}{A} \int e^{i\vec{G}\cdot\vec{r}} V(\vec{r}) d\vec{r} \quad if \quad \vec{k} - \vec{k}' = \vec{G}$$
(18.191)

or in terms of the integral over one primitive unit cell (PUC) of area Q as

$$V_{\vec{G}} = \frac{1}{Q} \int_{PUC} e^{i\vec{G}\cdot\vec{r}} V(\vec{r}) d\vec{r}$$
(18.192)

The strongly mixed states satisfying $\vec{k} - \vec{k}' = \vec{G}$ are those with wave vectors near Brillouin zone boundaries. All other states can be treated by perturbation theory. Let us be precise about what this statement means. If we introduce the periodic potential energy as a perturbation, we obtain an expression for the firstorder perturbed wave function in terms of the $\psi_{E,\vec{k}}^{(0)}(\vec{r})$ and a sum over all other free-electron wave functions with wave vectors $\vec{k}' = \vec{k} - \vec{G}$ for every reciprocal lattice translation vector \vec{G} (as we found earlier). If \vec{k} is not near a Brillouin zone boundary, all the other free-electron states mix weakly with $\psi^{(0)}_{E,\vec{k}}(\vec{r})$ and will not greatly affect the energy or wave function. If \vec{k} is near a zone boundary, one or more other states will mix strongly with $\psi_{E,\vec{k}}^{(0)}(\vec{r})$. These states satisfy the selection rule $\vec{k} - \vec{k}' = \vec{G}$ and have energies very close to each other $(|\vec{k}| \approx |\vec{k}'|)$ so that the energy denominator in the perturbation theory summation is small. Thus, at or near a single Brillouin zone boundary, two states are strongly mixed. At or near the intersection of two or more zone boundaries, more than two states can be strongly mixed. For example, if k is near the intersection of two boundaries, then we can associate two other equivalent wave vectors with \vec{k} , each of which corresponds to a state nearly degenerate with $\psi_{E,\vec{k}}^{(0)}(\vec{r})$. (Notice that this situation did not arise in one dimension). For example, in Figure 18.70 below, we show the location of several strongly mixed states for the first four Brillouin zones of the square lattice.



Figure 18.70: Strongly mixing states

In one case, \vec{k} is near a single zone boundary, and there is only one state that mixes strongly with $\psi_{E,\vec{k}}^{(0)}(\vec{r})$. In the other case shown, \vec{k} is near the intersection of three zone boundaries, and we must contend with four strongly mixed states. In Figure 18.70, the first four Brillouin zones of the square lattice in the reduced zone scheme are shown. The arrows connect the \vec{k} values for strongly mixed states. Two cases are considered, one near the edge of one zone boundary (two states) and one near the intersection of three boundaries (four states).

Calculation of Band Gaps

The calculation of the band gap for a two-dimensional crystal at any single Brillouin zone boundary is analogous to the one-dimensional calculation we did earlier. However, a somewhat more elaborate calculation is required when two or more Brillouin zone boundaries intersect.

Let us focus on one of these cases in the square lattice and calculate the energy gaps that arise from this strong mixing. In particular, suppose that we choose \vec{k} at the corner of the first Brillouin zone, $\vec{k} = (\pi/d)(1,1)$. At this point, three Brillouin zone boundaries intersect, so four free-electron states are strongly mixed. These states correspond to the \vec{k} vectors

$$(\pi/d)(1,1), (\pi/d)(1,-1), (\pi/d)(-1,1), (\pi/d)(-1,-1)$$
 (18.193)

and their negatives. In general, we can write these vectors as

$$\dot{G} = (2\pi/d) (m, n)$$
 (18.194)

and can denote $V_{\vec{G}}$ by V_{mn} .

The weak-binding wave function ψ_E^{weak} can be written as a linear combination of the strongly mixed free-electron wave functions

$$\psi_E^{weak}(\vec{r}) = \sum_{i=1}^4 a_i \psi_{E,i}^{(0)}(\vec{r})$$
(18.195)

where the $\psi_{E,i}^{(0)}(\vec{r})$ are the four free-electron wave functions corresponding to the wave vectors of above. (Remember that these four free-electron states are

degenerate). Substituting this expansion into the Schrodinger equation

$$\hat{H}\psi_E = E\psi_E \tag{18.196}$$

we obtain

$$\hat{H}\sum_{i=1}^{4} a_i \psi_{E,i}^{(0)}(\vec{r}) = E\sum_{i=1}^{4} a_i \psi_{E,i}^{(0)}(\vec{r})$$
(18.197)

The corresponding eigenvalue equation is obtained by multiplying this equation by $\psi_{E,j}^{(0)*}(\vec{r})$ and integrating over $d\vec{r} = dxdy$ (using orthonormality of the free-electron wave functions)

$$\sum_{i=1}^{4} H_{ji} a_i = E a_j \quad , \quad j = 1, 2, 3, 4$$
(18.198)

where H_{ji} is the matrix element

$$H_{ji} = \langle j | \hat{H} | i \rangle = \int d\vec{r} \psi_{E,j}^{(0)*}(\vec{r}) \hat{H} \psi_{E,i}^{(0)}(\vec{r})$$
(18.199)

This result yields the determinant equation

$$\det\left(H_{ji} - E\delta_{ji}\right) = 0 \tag{18.200}$$

For convenience, we will measure the energy from V_{00} , the constant part of the crystal potential energy (taken as the zero of energy in the free-electron approximation). The diagonal elements of the Hamiltonian matrix $(H_{ji}, i = j)$ are due solely to the free-electron term corresponding to the various \vec{k} values. Thus the determinant equation becomes

$$\frac{\frac{\hbar^{2}k^{2}}{2m_{e}} - E}{V_{01}} = V_{-10} V_{-10} V_{-1-1} V_{01} \frac{\frac{\hbar^{2}k^{2}}{2m_{e}} - E}{V_{-11}} V_{-10} V_{10} V_{10} V_{1-1} \frac{\frac{\hbar^{2}k^{2}}{2m_{e}} - E}{V_{0-1}} V_{11} V_{10} V_{0-1} \frac{\frac{\hbar^{2}k^{2}}{2m_{e}} - E}{V_{0-1}} = 0$$
(18.201)

where $k = \sqrt{2}(\pi/d)$. From an (18.191) or (18.192), V_{mn} is given by

$$V_{mn} = \frac{1}{d^2} \int_{PUC} \exp\left[i\left(\frac{2\pi}{d}mx + \frac{2\pi}{d}ny\right)\right] V(x,y) dxdy$$
(18.202)

Expanding the exponentials, we obtain

$$V_{mn} = \frac{1}{d^2} \int_{PUC} \cos \frac{2\pi}{d} mx \cos \frac{2\pi}{d} ny V(x, y) dx dy$$

$$+ \frac{1}{d^2} \int_{PUC} \left(-\sin \frac{2\pi}{d} mx \sin \frac{2\pi}{d} ny + i \cos \frac{2\pi}{d} mx \sin \frac{2\pi}{d} ny \\ + i \sin \frac{2\pi}{d} mx \cos \frac{2\pi}{d} ny \right) V(x, y) dx dy$$
(18.203)

Clearly, we must know more about the form of V(x, y) in order to further evaluate this matrix element. Since the crystal potential energy has fourfold rotational symmetry, it satisfies

$$V(x,y) = V(y,-x) = V(-x,-y) = V(-y,x)$$
(18.204)

If we consider only a square crystal with mirror symmetry such that

$$V(x,y) = V(-x,y) = V(x,-y)$$
(18.205)

the second integral in the expression for V_{mn} is zero, and we conclude that

$$V_{mn} = V_{n-m} = V_{-m-n} = V_{-nm}$$
(18.206)

Using this result, we can define two real quantities V_1 and V_2 by

$$V_1 = V_{10} = V_{0-1} = V_{-10} = V_{01}$$
, $V_2 = V_{11} = V_{1-1} = V_{-1-1} = V_{-11}$ (18.207)

Let us also define a quantity ε equal to the actual energy as measured from the free-electron value,

$$\varepsilon = E - \frac{\hbar^2 k^2}{2m_e} \tag{18.208}$$

Written in terms of $V_1,\,V_2$ and ε , the determinant equation takes on the far simpler form

$$\varepsilon^{4} - 2(2V_{1}^{2} + V_{2}^{2})\varepsilon^{2} - 8V_{1}^{2}V_{2}\varepsilon + V_{2}^{2}(-4V_{1}^{2} + V_{2}^{2}) = 0$$
(18.209)

Factoring this equation, we have

$$(\varepsilon + V_2)^2 (\varepsilon - V_2 + 2V_1) (\varepsilon - V_2 - 2V_1) = 0$$
(18.210)

This equation is a quartic equation, so it has four roots. The eigenvalues are

$$E = \begin{cases} \frac{\hbar^2 k^2}{2m_e} - V_2 & \text{twice} \\ \frac{\hbar^2 k^2}{2m_e} + V_2 \pm V_1 \end{cases}$$
(18.211)

These are the energies of the four weak-binding states whose wave functions are given by the linear combinations above. They arise from the mixing of four freeelectron states at the corner $\vec{k} = (\pi/d) (1, 1)$ of the first Brillouin zone. Notice that a twofold degeneracy remains in the weak-binding approximation.

E versus Path Distance

We can usually assume that $|V_2| < |V_1|$, that is, that the matrix elements are smaller for longer \vec{G} vectors. Then we obtain four energies at the corner of the first Brillouin zone, one above and one below a pair of degenerate levels.

This result induces gaps in the E versus path distance plot for the square lattice (remember that our earlier plot had no gaps). The modified plot of weak-binding energy versus path distance for paths of the first four bands of the square lattice (energy is shown in reduced units) is shown in Figure 18.71 below. The bands are labeled.



Figure 18.71: Band Gaps create Distinct Bands

Compare this plot to the earlier plot in Figure 18.69.

Here splittings appear between every band for all values of \vec{k} except at the zone corner. But values of E do not exist for which no electronic states are allowed, that is, there are no actual band gaps. In fact, the bands overlap in this example. These features are characteristic of two- (and three-) dimensional systems.

Constant Energy Contours

We have seen that only near a Brillouin zone boundary is the weak-binding energy appreciably different from the free-electron energy. Consequently, we expect that, in the weak-binding approximation, constant energy contours for a two-dimensional lattice would be altered significantly from the free-electron contours we described earlier only near a zone boundary. For any given wave vector \vec{k} ear a single zone boundary, the energy in the weak-binding approximation is lower than the free-electron energy if \vec{k} is *inside* the zone boundary. Energies for \vec{k} outside the Brillouin zone boundary are raised from their freeelectron values due to the mixing of the two free-electron states. In addition, if we are close to only one zone boundary, the constant energy contours will strike the boundary at a right angle. These effects *bend* the contours in toward the boundaries, as shown in Figure 18.72 below.



Figure 18.72: Constant energy contours bending toward zone boundaries

Above, we have shown a comparison of a weak-binding constant energy contour (solid curve) and a free-electron constant energy contour (dashed curve) near a Brillouin zone boundary.

Returning to the square lattice, we show in Figure 18.73 below how to modify the free-electron constant energy contours. Contours are shown in the weakbinding approximation for the first four bands in the reduced zone scheme.



Figure 18.73: Modified constant energy contours

Fermi Surfaces

The Fermi surfaces are simply particular constant energy contours corresponding to the Fermi energies. Fermi surfaces for several values of η shown in Figure 18.74 below. These curves are obtained by modifying the surfaces we drew earlier, using the bending at the boundary method shown above.



Figure 18.74: Fermi surfaces for $\eta = 1$

For a crystal with a square lattice and $\eta = 1$, the Fermi surface in the weakbinding approximation is a circle whose area is half that of the first zone. Since this circle is far from the zone boundaries, it is unaltered from its free-electron behavior. This feature is not true of other values of η , as the figure shows.

18.7 Born-Oppenheimer description of two atoms in a combined oscillator and lattice trap

In this section, we analyze the quantum states of two atoms in a combined harmonic oscillator and periodic lattice trap in one spatial dimension. In the case of tight-binding and only nearest neighbor tunneling, the equations of motion are conveniently represented in the momentum representation. We then show that in the case of strong attraction between the particles, the different time scales of relative and center-of- mass motion validate a separation of the problem similar to the Born-Oppenheimer approximation applied in the description of electronic and nuclear motion in molecules.

18.7.1 Introduction

We will now study cold atoms(lattice trap) in periodic potentials formed by standing wave laser beams.

18.7.2 Lattice Hamiltonian

A. One-body Hamiltonian and Wannier states

We consider a particle moving in a sinusoidal potential, so that the Hamiltonian can be written

$$\hat{H}_{lat} = \hat{P}^2 + V_0 \sin^2\left(\pi \hat{X}\right) \tag{18.212}$$

where the scaled position and momentum operators have the dimensionless commutator

$$[\hat{X}, \hat{P}] = i$$
 (18.213)

Since the potential is periodic with unit period, Bloch's theorem ensures that we can choose energy eigenstates

$$\hat{H}_{lat} \left| \psi_q^{(n)} \right\rangle = E_q^{(n)} \left| \psi_q^{(n)} \right\rangle \tag{18.214}$$

with quasi-momenta $q \in [-\pi, \pi]$ and band indices $n = 0, 1, \dots$ Another basis - the Wannier states -can be obtained as the Fourier transform over a single Brillouin zone of the eigenstates

$$\left|w_{k}^{(n)}\right\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{+\pi} dq e^{-ikq} \left|\psi_{q}^{(n)}\right\rangle$$
 (18.215)

For sufficiently deep lattices, the Wannier states with different n are localized around different lattice potential minima and are identical up to translation. We note that, within each energy band, the overlap between the quasi-momentum eigenstates and the Wannier states

$$\left(\psi_q^{(n)} \left| w_k^{(n)} \right\rangle = \frac{\delta_{m,n}}{\sqrt{2\pi}} e^{-ikq} \tag{18.216}$$

is similar to the usual overlap between position eigenstates and momentum eigenstates.

The Hamiltonian is block-diagonal in the basis of Wannier states, and the coupling of Wannier states at different locations is given by

$$\left(w_{k}^{(m)}\middle|\hat{H}_{lat}\middle|w_{k}^{(n)}\right) = \delta_{m,n}J_{|j-k|}^{(n)}$$
 (18.217)

where

$$J_k^{(n)} = -\frac{1}{2\pi} \int_{-\pi}^{+\pi} dq e^{ikq} E_q^{(n)}$$
(18.218)

This shows that $J_k^{(n)}$ is the Fourier transform of the energy bands as a function of q and the dispersion relations can be written as

$$E_q^{(n)} = -\sum_{k=0}^{\infty} J_k^{(n)} e^{-ikq} = -J_0^{(n)} - 2\sum_{k=1}^{\infty} J_k^{(n)} \cos\left(kq\right)$$
(18.219)

For deep potentials the energy bands are relatively flat, and the higher order cosine terms are suppressed. This justifies the tight binding approximation in which one retains only the nearest lattice site coupling, and in the following we will suppress the band index (n), and focus on the lowest band described by the tight binding Hamiltonian

$$\hat{H}_{TB} = -J_1 \sum_{k=-\infty}^{\infty} \{ |w_{k-1}\rangle \langle w_k| + |w_{k+1}\rangle \langle w_k| \}$$

= $-2J_1 \cos{(\hat{P})}$ (18.220)

B. Harmonic confinement

Adding a harmonic confinement to the lattice potential is adequately described by adding the term $k\hat{X}^2$ with the spring constant k to the Hamiltonian. For deep lattice potentials, the Wannier state $Ketw_j$ is well localized at X = j, so we make the approximation to replace \hat{X} by the discrete quasi-position operator of the lowest band

$$\hat{W} = \sum_{j=-\infty}^{\infty} j |w_j\rangle \langle w_j| \qquad (18.221)$$

Introducing a rescaling of the Hamiltonian by $4J_1$ and defining $\kappa=k/4J_1$ we end up with the Hamiltonian

$$\hat{H} = \frac{\hat{H}_{TB}}{4J_1} + \frac{k\hat{W}^2}{4J_1} = \kappa\hat{W}^2 - \frac{\cos\left(\hat{P}\right)}{2}$$
(18.222)

Similar to the usual relationship between continuous position and momentum operators, the discrete position operator \hat{W} acts as a differentiation in the continuous quasi-momentum representation

$$\langle \psi_q | \hat{W} | \alpha \rangle = i \frac{\partial}{\partial q} \langle \psi_q | \alpha \rangle$$
 (18.223)

which is easily derived by inserting a resolution of the identity in Wannier states and using the overlap formula (18.216). Therefore, we arrive at the quasimomentum expression of the single particle Hamiltonian

$$\left\langle \psi_{q} \right| \hat{H} \left| \alpha \right\rangle = \left(-\kappa \frac{\partial^{2}}{\partial q^{2}} - \frac{\cos\left(q\right)}{2} \right) \left\langle \psi_{q} \right| \alpha \right\rangle \tag{18.224}$$

At this point we make the curious observation that, after having restricted the Hilbert space to the lowest energy band and having added a quasi-harmonic confinement, the Hamiltonian in momentum space (18.224) has the same form as the original optical lattice Hamiltonian (18.214) in position space. In both cases, the Schrödinger equation takes the form of the Mathieu equation, but instead of looking for eigenstates of (18.214) with any quasi-momentum, we will only look for periodic eigenstates for (18.224), i.e. with zero "quasi-position". C. Interacting particles

In an ultra-cold gas of bosons, the interaction between the particles is adequately described by the two-particle contact interaction operator \hat{U}_{int} with the matrix elements

$$\langle X_1; X_2 | \hat{U}_{int} | X_3; X_4 \rangle = g\delta(X_1 - X_3)\delta(X_2 - X_4)\delta(X_3 - X_4)$$
(18.225)

for some interaction strength g. In the tight binding approximation, the Wannier states are localized at different lattice sites, and one may neglect matrix elements of the interaction potential with Wannier product states located on different sites. We thus end up with the following effective interaction operator acting on two-particle states

$$\hat{U}_{int}^{eff} = G \sum_{j} |w_j; w_j\rangle \langle w_j; w_j|$$
(18.226)

where the strength parameter is given by

$$G = g \int dX \left| w_0(X) \right|^4 \tag{18.227}$$

Using the relation (18.216), we can calculate the matrix elements of the effective interaction operator in quasi-momentum space

$$\langle \psi_{q_1}; \psi_{q_2} | \hat{U}_{int}^{eff} | \psi_{q_3}; \psi_{q_4} \rangle = \frac{G}{2\pi} \delta(q_3 + q_4 - q_1 - q_2)$$
(18.228)

which shows that the interaction conserves the total quasi-momentum and is independent of its value.

A system of two identical particles in an optical lattice with harmonic confinement, which interact by the contact interaction is described by the Hamiltonian

$$\hat{H} = \kappa (\hat{W}_1^2 + \hat{W}_2^2) - \frac{\cos(\hat{P}_1)}{2} - \frac{\cos(\hat{P}_2)}{2} + \hat{U}$$
(18.229)

with $\hat{U} = \hat{U}_{int}^{eff}/4J_1$.

18.7.3 Relative- and Center-of-Mass Quasi-Momenta

In the quasi-momentum representation

$$\frac{\cos\left(\hat{P}_{1}\right) + \cos\left(\hat{P}_{2}\right)}{2} |\psi_{q_{1}};\psi_{q_{2}}\rangle$$

$$= \frac{\cos\left(q_{1}\right) + \cos\left(q_{2}\right)}{2} |\psi_{q_{1}};\psi_{q_{2}}\rangle$$

$$= \cos\left(\frac{q_{1} + q_{2}}{2}\right) \cos\left(\frac{q_{1} - q_{2}}{2}\right) |\psi_{q_{1}};\psi_{q_{2}}\rangle$$

$$\equiv \cos\left(\frac{\hat{Q}_{+}}{2}\right) \cos\left(\frac{\hat{Q}_{-}}{2}\right) |\psi_{q_{1}};\psi_{q_{2}}\rangle \qquad (18.230)$$

where we have defined new operators by their action on quasi-momentum eigenstates,

$$q^{iQ_{\pm}/2} |\psi_{q_1}; \psi_{q_2}\rangle \equiv e^{i(q_1+q_2)/2} |\psi_{q_1}; \psi_{q_2}\rangle \tag{18.231}$$

The introduction of these operators suggest to reparameterize the quasi-momentum basis states $|\psi_{q_1}; \psi_{q_2}\rangle$ in terms of their sum and difference:

$$q_{\pm} = q_2 \pm q_1 \tag{18.232}$$

The quasi-momentum eigenstates states are defined for pairs of q_1 and q_2 in the set

$$S_{12} = [-\pi; \pi] \times [-\pi; \pi]$$
(18.233)

corresponding to a diamond shaped area in the coordinate plane of q_{\pm} as shown in figure 18.75 below.



Figure 18.75: Quasi-momentum of the two particles vs. relative and center-ofmass quasi-momentum. Left: The first Brillouin zone S_{12} in the (q_1, q_2) -plane is emphasized and repeated in each direction. The color coding indicates the values of a function that is periodic in both variables with period 2π and illustrates the required periodicity. The set S_{\pm} which contains exactly one representative of each point from S_{12} is shown by the gray rectangle. Right: The same function is shown but in the (q_+, q_7) -coordinate system. The set S_{\pm} is emphasized and repeated, but with a different tiling than for S_{12} in the left panel.

If we choose the values of $(q_+, q_?)$ in the set

$$S_{\pm} = [-\pi; \pi] \times [-2\pi; 2\pi]$$
(18.234)

then each point from S_{12} is represented exactly once as is evident from figure 18.75. This means that we can reparametrize the quasi-momentum eigenstates as

$$|q_{+},q_{-}\rangle = \frac{1}{\sqrt{2}} |\psi_{(q_{+}-q_{-})/2};\psi_{(q_{+}+q_{-})/2}\rangle$$

$$|\psi_{q_{1}};\psi_{q_{2}}\rangle = \sqrt{2} |q_{1}+q_{2},q_{2}-q_{1}\rangle$$
(18.235)

where the front factor is chosen to preserve orthonormality, such that we have the resolution of identity

$$\hat{1} = \int_{-\pi}^{+\pi} dq_{+} \int_{-2\pi}^{+2\pi} dq_{-} |q_{+}, q_{-}\rangle \langle q_{+}, q_{-}| \qquad (18.236)$$

The corresponding discrete relative and center-of-mass position coordinates

$$\hat{W}_{\pm} \equiv \frac{\hat{W}_2 + \hat{W}_1}{2} \tag{18.237}$$

act in the following way

$$\langle q_{+}, q_{-} | \hat{W}_{\pm} | \alpha \rangle = i \frac{\partial}{\partial q_{\pm}} \langle q_{+}, q_{-} | \alpha \rangle$$
(18.238)

and the interaction operator \hat{U} has the following matrix elements in terms of the relative and center-of-mass quasi-momentum states

$$\langle q_{+}, q_{-} | \hat{U} | \alpha \rangle = \gamma \int_{-2\pi}^{+2\pi} dq'_{-} \langle q_{+}, q'_{-} | \alpha \rangle$$
 (18.239)

with $\gamma = G/(16\pi J_1)$.

The two-atom Hamiltonian can now be written,

$$\hat{H} = 2\kappa (\hat{W}_{+}^{2} + \hat{W}_{-}^{2}) - \cos\left(\frac{\hat{Q}_{+}}{2}\right) \cos\left(\frac{\hat{Q}_{-}}{2}\right) + \hat{U}$$
(18.240)

The Schrodinger equation with the Hamiltonian (18.240) can be solved accurately for a wide range of parameters as in 18.241 below. The resulting eigenenergies and the wave functions (18.246 below) will be used as reference for our analysis by the Born-Oppenheimer separation of the motional degrees of freedom.

Solving the equations numerically

1. Solving the non-approximated equation

To solve the two-atom Schrodinger equation in the tight binding approximation we expand the state as

$$|\alpha\rangle = \sum_{j,k} F_{j,k} |w_j; w_k\rangle \tag{18.241}$$

The stationary Schrodinger equation with the Hamiltonian (18.240) yields the equation for the expansion coefficients

$$EF_{j,k} = 4\pi\gamma\delta_{j,k}F_{j,k} + \kappa(j^2 + k^2)F_{j,k} - \frac{F_{j-1,k} + F_{j+1,k} + F_{j,k-1} + F_{j,k+1}}{4}$$
(18.242)

The original Hamiltonian is invariant under parity inversion of both particles so we can find a complete set of solutions of even and odd wave-functions. In terms of the expansion (18.241) this means that we can find solutions where

$$F_{-j,-k} = pF_{j,k} \tag{18.243}$$

where p can assume the values ± 1 . In addition, since we are dealing with two identical bosons, only symmetrized wave functions are physically meaningful, with implies that we have the symmetry

$$F_{j,k} = F_{k,j}$$
 (18.244)

For numerical purposes we enforce these requirements by hand in the following way. Instead of looking at all pairs $(j, k) \in \mathbb{Z}^2$, we restrict our attention to those in the subset

$$T = \{(j,k) \in \mathbb{Z}^2 ||k| \le j \le j_{max}\} \subset \mathbb{Z}^2$$
(18.245)

for some manually chosen j_{max} . Using the symmetries we reformulate the recurrence equation such that it only involves coefficients from T. The equation can be expressed as a matrix eigenvalue equation which is amenable to standard numerical diagonalization routines. When all coefficients have been found - and properly normalized - the wave function in relative and center-of-mass quasimomenta is given by

$$\langle q_+, q_- | \alpha \rangle = \sum_{j,k} F_{j,k} \langle q_+, q_- | w_j; w_k \rangle$$

= $\frac{1}{\sqrt{2}(2\pi)} \sum_{j,k} F_{j,k} e^{-i(j+k)q_+/2} e^{-i(k-j)q_-/2}$ (18.246)

18.7.4 Born-Oppenheimer Separation

A. Derivation

We write the Hamiltonian in (18.240) as

$$\hat{H} = \hat{H}_{-} + 2\kappa \hat{W}_{+}^{2} \tag{18.247}$$

where

$$\hat{H}_{-} = 2\kappa \hat{W}_{-}^{2} - \cos\left(\frac{\hat{Q}_{+}}{2}\right) \cos\left(\frac{\hat{Q}_{-}}{2}\right) + \hat{U}$$
(18.248)

We note that $e^{i\hat{Q}_+/2}$ commutes with \hat{H}_- and we define their joint eigenstates by $|q_+,n\rangle$:

$$H_{-}|q_{+},n\rangle = \epsilon_{n}(q_{+})|q_{+},n\rangle$$
 (18.249)

$$e^{i\hat{Q}_{+}/2}|q_{+},n\rangle = e^{iq_{+}/2}|q_{+},n\rangle$$
 (18.250)

with the following orthogonality relations

$$\langle q_+, n | q'_+, n' \rangle = \delta_{n,n'} \delta(q_+ - q'_+)$$
 (18.251)

The states $|q_+, n\rangle$ can be expanded

$$|q_{+},n\rangle = \int_{-2\pi}^{+2\pi} dq'_{-} A_{n}^{(q_{+})}(q'_{-}) |q_{+},q_{-}\rangle$$
(18.252)

and the orthogonality relation (18.251) implies

$$\int_{-2\pi}^{+2\pi} dq_{-} \left[A_{n}^{(q_{+})}(q_{-}) \right]^{*} A_{n'}^{(q_{+})}(q_{-}) = \delta_{n,n'}$$
(18.253)

Any eigenstate of the full Hamiltonian (18.247) can be expanded as

$$|\psi\rangle = \int_{-\pi}^{+\pi} dq'_{+} \sum_{n} C^{(n)}(q'_{+}) |q'_{+}, n\rangle$$
(18.254)

The expansion coefficients $C^{(n)}(q'_{+})$ are found by applying the Hamiltonian (18.247) to the expanded wave function (18.254) and using (18.248)

$$\hat{H} |\psi\rangle = \int_{-\pi}^{+\pi} dq'_{+} \sum_{n} C^{(n)}(q'_{+}) \{\epsilon_{n}(q'_{+}) + 2\kappa \hat{W}_{+}^{2}\} |q'_{+}, n\rangle$$
(18.255)

In the $(q_+, q_?)$ -representation for the state vector, the eigenvalue equation takes the form of coupled differential equations

$$E\sum_{n} A_{n}^{(q_{+})}(q_{-})C^{(n)}(q'_{+})$$

$$=\sum_{n} \left\{ \epsilon_{n}(q'_{+}) - 2\kappa \frac{\partial^{2}}{\partial q_{+}^{2}} \right\} A_{n}^{(q_{+})}(q_{-})C^{(n)}(q'_{+})$$
(18.256)

The goal of the following analysis is to find an approximation for the eigenstates, which is easier to apply numerically and which offers insights into their internal structure and dynamics. To this end, we assume that the states $|q'_{+}, n\rangle$ described by q_{-} wave functions $A_n^{(q_{+})}(q_{-})$ depend only weakly on the argument q_{+} . Eliminating thus the partial derivatives of $A_n^{(q_{+})}(q_{-})$ with respect to q_{+} in the evaluation of the right hand side of (18.256), and using the orthogonality of the $A_n^{(q_+)}(q_-)$ functions, we arrive at the following approximate equation for the expansion coefficients

$$\epsilon_n(q_+)C^{(n)}(q_+) - 2\kappa \frac{\partial^2 C^{(n)}(q_+)}{\partial q_+^2} = EC^{(n)}(q_+)$$
(18.257)

This has the form of a Schrodinger equation for a single particle in the potential $\epsilon_n(q_+)$. For each energy potential we can find discrete eigenenergies $E_m^{(n)}$ and associated eigenfunctions $C_m^{(n)}$ that solve (18.257) and yield approximate eigenstates $|\psi_m^{(n)}\rangle$ for the full Hamiltonian (18.247)

$$\langle q_+, q_- | \psi_m^{(n)} \rangle = C_m^{(n)}(q_+) A_n^{(q_+)}(q_-)$$
 (18.258)

Note the formal similarity of this reduction of the problem with the use of the Born-Oppenheimer approximation in chemistry. In the latter, the wave function is expanded as a product of wave functions in nuclear and electronic coordinates, and due to the large difference in mass and hence in energy and time scales, the electronic wave functions are supposed to follow changes in the slow nuclear coordinates adiabatically.

In our case, the two particles have identical masses, and in the absence of mutual interaction, the relative and center-of-mass motion occur on similar time scales, and the Born-Oppenheimer approximation should not be valid. But, as we increase the attractive interaction between the atoms, bounds states are formed, and the relative position develops a new, faster time scale given by the binding energy. Our separation is carried out and motivated in the quasi-momentum picture, where a further observation may be in order: a strongly bound state in the relative position coordinate corresponds to a very extended wave function in the relative momentum, while the center-of-mass momentum may be well defined. This supports the assumption that the dominant contribution to the second derivative in (18.256) stems from the q_+ wave function $C_m^{(n)}(q_+)$, and hence that the derivative of $A_n^{(q_+)}$ with respect to q_+ may be neglected.

B. Application

Before we apply the Born-Oppenheimer approximation, let us consider how we expand states onto the center-of-mass and relative quasi-momentum eigenstates. Every state can be expanded in both the two-particle quasi-momentum basis, and in the basis of relative and center-of-mass quasi-momenta.

$$|\phi\rangle = \begin{cases} \int_{-\pi}^{+\pi} dq_1 \int_{-\pi}^{+\pi} dq_2 \alpha(q_1, q_2) |\psi_{q_1}; \psi_{q_2}\rangle \\ \\ \int_{-\pi}^{+\pi} dq_+ \int_{-2\pi}^{+2\pi} dq_- \beta(q_+, q_-) |q_+, q_-\rangle \end{cases}$$
(18.259)

While $|q_1, q_2\rangle$ and $|q_+, q_-\rangle$ are defined for $(q_1, q_2) \in S_{12}$ and $(q_+, q_-) \in S_{\pm}$, respectively, we can look for functions defined on the entire \mathbb{R}^2 and restrict the

solution afterwards. The function α is periodic in both variables with period 2π , and this enforces β to obey the symmetry

$$\beta(q_+ + 2\pi, q_- \pm 2\pi) = \beta(q_-, q_-) \tag{18.260}$$

c.f. the tiling of \mathbb{R}^2 with replicas of S_{\pm} in the right panel of figure 18.75. Thus, a necessary - but not sufficient - condition is that β is periodic in both q_+ and $q_$ with periodicity 4π . We are considering bosons and the state must be symmetric under the exchange of the two particles, $(q_+, q_-) \mapsto (q_+, -q_-)$, which implies the further constraint

$$\beta(q_+, q_-) = \beta(q_+, -q_-) \tag{18.261}$$

Using these arguments on (18.258) we conclude that we are looking for solutions such that $A_n^{(q_+)}(q_-)$ is even and periodic in q_- with period 4π , and such that the *product* of $C_m^{(n)}(q_+)$ and $A_n^{(q_+)}(q_-)$ is periodic in q_+ with the same period. Furthermore, the product must satisfy the relation (18.260).

1. The first Born-Oppenheimer equation

To apply the Born-Oppenheimer approximation, we must first find the eigenstates of \hat{H}_{-} and their eigenenergies, and using the formal expansion of the states (18.252), the eigenvalue equation (18.249) leads to the equation

$$\epsilon_{n}(q_{+})A_{n}^{(q_{-})} = \left[-2\kappa \frac{\partial^{2}}{\partial q_{-}^{2}} - F(q_{+})\cos\left(\frac{q_{-}}{2}\right)\right]A_{n}^{(q_{+})}(q_{-}) + \gamma \int_{-2\pi}^{+2\pi} dq'_{-}A_{n}^{(q_{+})}(q_{-})$$
(18.262)

where $F(q_+) = \cos\left(\frac{q_+}{2}\right)$. For each value of q_+ this equation has the form of a Schrödinger equation with argument q_- , and with a periodic $\cos\left(\frac{q_-}{2}\right)$ potential with amplitude $F(q_+)$ and a non-local potential with strength γ . Solutions which are periodic in q_- with period 4π are readily found by Fourier expansion of $A_n^{(q_+)}(q_-)$ as in 18.246.

When solving (18.262) we are looking for solutions to a Schrodinger like equation with a cosine potential with period 4π . Solutions which are periodic with the same period - referred to as zero quasi-momentum states for periodic problems in position space - can be chosen to be real-valued. The front factor $F(q_+)$ of the cosine potential is itself a cosine function of q_+ leading to two observations:

1. $F(q_+)$ is an even function of q_+ so equation 18.262 is unaltered under the transformation $q_+ \mapsto -q_+$. Thus the solutions must be identical up to a complex factor, and since they are real-valued we can choose the solutions as

$$A_n^{(q_+)}(q_-) = A_n^{(-q_+)}(q_-)$$
(18.263)

We could not have chosen a minus sign, since this would have made $A_n^{(q_+)}$ vanish for $q_+ = 0$.

2. $F(q_+)$ changes to values of opposite sign when q_+ is increased by an amount of 2π and the cosine potential $\cos(q_-/2)$ in (18.262) is effectively translated by half a period. For this translated potential the eigenvalues are the same, while the eigenfunctions are translated and scaled

$$\epsilon_n(q_+) = \epsilon_n(q_+ + 2\pi) \tag{18.264}$$

$$A_n^{(q_+)}(q_-) = \xi_n A_n^{(q_++2\pi)}(q_- \pm 2\pi)$$
(18.265)

The factor ξ_n may take the values $\pm 1 \sin A_n^{(q_+)}(q_-)$ is real-valued for all values of q_+ and q_- .

Applying the relations (18.263) and (18.265) for $q_{+} = -\pi$ we get the relation

$$A_n^{(+\pi)}(q_-) = \xi_n A_n^{(+\pi)}(q_- \pm 2\pi)$$
(18.266)

so we can determine ξ_n from the translational symmetries of $A_N^{(+\pi)}$.

2. The second Born-Oppenheimer equation

Eq. (18.262) yields the potential $\epsilon_n(q_+)$ which is periodic with period 2π , and we are looking for functions $C_m^{(n)}(q_+)$ that are periodic in q_+ with period 4π . Therefore, Bloch's theorem tells us that we can choose a complete set of solutions as

$$C_m^{(n)}(q_+) = e^{i\delta_n q_+/2} D_m^{(n)}(q_+)$$
(18.267)

where $D_m^{(n)}$ is periodic with period 2π , and $\delta_n = 0, 1$. For $\delta_n = 0$ the solution $C_m^{(n)}(q_+)$ is thus periodic with period 2π , whereas for $\delta_n = 1$, it is antiperiodic. We require that the product of $C_m^{(n)}(q_+)$ and $A_n^{(q_+)}(q_-)$ satisfies the symmetry (18.260), and if we combine this with (18.265), we get the relation

$$C_m^{(n)}(q_+)A_n^{(q_+)}(q_-) = \xi_n C_m^{(n)}(q_+ + 2\pi)A_n^{(q_+)}(q_-)$$
(18.268)

from which we conclude that $C_m^{(n)}(q_+)$ must fulfill the symmetry

$$C_m^{(n)}(q_+ + 2\pi) = \xi_n C_m^{(n)}(q_+) A_n^{(q_+)}$$
(18.269)

Comparing to (18.267) we see that this implies that for $\xi_n = -1$ we must choose $\delta_n = 1$ and for $\xi_n = +1$, we can use $\delta = 0$. We can solve (18.257) by a Fourier expansion of $D_m^{(n)}$ and ϵ_n (as shown below in 18.270).

2. Solving the first Born-Oppenheimer equation

The solutions of (18.262) are functions $A_n^{(q_+)}(q_-)$ which are periodic in q_- with period 4π . Therefore, for each value of q_+ we make the expansion

$$A_n^{(q_+)}(q_-) = \frac{1}{\sqrt{4\pi}} \sum_j \alpha_{j,n}^{(q_+)} e^{ijq_-/2}$$
(18.270)

and obtain the tridiagonal recurrence relation,

$$\frac{F(q_{+})}{2} \left[\alpha_{j-1,n}^{(q_{+})} + \alpha_{j+1,n}^{(q_{+})} \right] \\ = \left(\frac{\kappa}{2} j^{2} + 4\pi \gamma \delta_{j,0} - \epsilon_{n}(q_{+}) \right) \alpha_{j,n}^{(q_{+})}$$
(18.271)

To accommodate the bosonic nature of the particles, we only look for even solutions to (18.262), so we only need to consider terms $\alpha_{j,n}^{(q_+)}$ with $j \ge 0$, and for j = 0 we use

$$F(q_{+})\alpha_{1,n}^{(q_{+})} = [4\pi\gamma - \epsilon_{n}(q_{+})]\alpha_{0,n}^{(q_{+})}$$
(18.272)

By expressing the recurrence relation as a matrix eigen-value equation, this can be truncated and solved with good accuracy.

2. Solving the Second Born-Oppenheimer equation

We solve the second Born-Oppenheimer equation using the results from the first Born-Oppenheimer equation. First, coefficients in the expansion

$$\epsilon_n(q_+) = \sum_k \beta_K^n e^{ijq_+} \tag{18.273}$$

are determined by a discrete Fourier transformation. We then use the expansion

$$C_m^{(n)}(q_+) = \frac{1}{\sqrt{2\pi}} \sum_l \gamma_l^{m,n} e^{i\left(l + \frac{\delta_n}{2}\right)q_+}$$
(18.274)

in (18.257) together with the expansion (18.273) which yields the following equation for the γ -coefficients

$$\sum_{k} \beta_k^n \gamma_{l-k}^{m,n} + 2\kappa \left(l + \frac{\delta_n}{2} \right)^2 \gamma_l^{m,n} = E_m^{(n)} \gamma_l^{m,n} \tag{18.275}$$

Since the potential energy curves $\epsilon_n(q+_+)$ are even functions, the solutions can be chosen to be either even or odd, and the coefficients then fulfill $\gamma_l^{m,n} = \pm \gamma_{-l}^{m,n}$. It suffices to only consider coefficients with $m \ge 0$ and solve the recurrence equations.

18.7.5 Exact and Born-Oppenheimer Approximate Solutions

A. Wave functions

When solving the first Born-Oppenheimer equation (18.256) we find eigenvalues $\epsilon_n(q_+)$ and eigenfunctions $A_n^{(q_+)}(q_-)$ for each value of $q_+ \in [-\pi, \pi]$. In the left-most panel in figure 18.76 below is shown the lowest few potential curves $\epsilon_n(q_+)$. The lowest potential curve is well separated from the higher ones which

lie closer. Each of the potential curves has an energy variation which is typically small compared to the energy distance between the bands. In the upper panels, a magnified view of the curves are shown. In the lower panels eigenfunctions $A_n^{(q_+)}(q_-)$ to the first Born-Oppenheimer equation are shown for four different values of n.



Figure 18.76: Energies and eigenfunctions found by solving the two Born-Oppenheimer equations for $\kappa = 0.5$ and $\gamma = -0.5$. Left panel: The six lowest potential curves $\epsilon_n(q_+)$ found from the first Born-Oppenheimer equation. Upper panels: Magnification of four of the potential curves in the left panel. Lower panels: Eigenfunctions $A_n^{(q_+)}(q_-)$ for the first Born-Oppenheimer equation shown for all values of q_+ for the corresponding *n*-values. In the upper panels are shown (horizontal dashed blue/red lines) the two lowest energies $E_j^{(n)}$ for j = 1, 2 found from solving the second Born-Oppenheimer equation in the potential $\epsilon_n(q_+)$ and the corresponding wave functions (solid blue/red lines).

The second Born-Oppenheimer equation uses the energies $\epsilon_n(q_+)$ as potential functions in a Schrodinger like equation, and each of the upper panels in Figure 18.76 show the energy levels of the two lowest eigenstates (m = 1, 2) in these potentials along with their eigenfunctions $C_m^{(n)}(q_+)$. As we saw in the previous section, the function $C_m^{(n)}(q_+)$ should be chosen periodic or anti-periodic depending on the value of ξ_n . By studying the behavior of $A_n^{(q_+)}(q_-)$ at $q_+ = \pm \pi$ one can see if ξ_n is +1 or -1 depending on whether the wave function $A_n^{(q_+)}(q_-)$ changes sign when translated by π or not. For n = 0, 2 the solutions $C_m^{(n)}(q_+)$ to the second Born-Oppenheimer equation must be periodic with period 2π , while for n = 1, 5 the solutions $C_m^{(n)}(q_+)$ must be chosen *anti*periodic.

Total Born-Oppenheimer solutions to the two-atom Hamiltonian are shown in Fig. 18.77 Panels (A1-2) corresponds to the approximate solutions from the n = 0 case of figure 18.76, panels (A3-4) corresponds to the n = 1 case, and panels (A5-6) corresponds to the n = 2 case. In the lower panels of figure 18.77 the corresponding exact two-atom eigenstates are shown. There is a good agreement between the exact and approximate solutions, especially for the low excitations of the lowest bands.



Figure 18.77: Upper panels: Quasi-momentum wave functions found by the Born-Oppenheimer approximation for $\kappa = 0.5$ and $\gamma = -0.5$. Columns 1-2 show the two lowest eigenstates in the lowest potential curve $\epsilon_0(q_+)$ corresponding to the n = 0 column in figure 18.76. Columns 3-4 correspond to the n = 1 column in figure 18.76 and columns 5-6 correspond to the n = 2 column in figure 18.76. Lower panels: The corresponding exact solutions.

B. Energies

In figure 18.78 both the exact and the approximative energies are shown for fixed κ as functions of the scaled interaction strength γ . Except in the region where γ is numerically small, there is reasonable agreement between the exact and the approximated energy levels. For negative γ there is a clear grouping of the energy levels in two groups: Those that are nearly constant as a function of

 γ and those that depend linearly on γ . Comparing to the approximate energies found by the Born-Oppenheimer approximation we see that the linear dependence comes from the fact that the position of the lowest potential curve varies linearly with γ .



Figure 18.78: Exact and approximate energies as a function of γ for $\kappa = 1$. Exact energies are plotted by the black dashed lines, and or n = 0, 1, 2, 3 the energies $E_j^{(n)}$ found from the Born-Oppenheimer equation is plotted in four different colors.

C. Approximate solution of the first Born-Oppenheimer equation

To understand the behavior of the energy spectra, we start by analyzing the system in the limit where at least one of the two coefficients γ, κ is (numerically) much larger than unity, so that we can find analytical approximations. This limit enables us to treat the term

$$-F(q_+)\cos\left(\frac{q_-}{2}\right) \tag{18.276}$$

in the first Born-Oppenheimer equation (18.256) as a perturbation. When we neglect this term, we can choose a complete set of eigenfunctions as plane waves with wave number k/2 for $k = 1, \pm 1, \pm 2, \ldots$ and with energies

$$\tilde{\epsilon}_k = \frac{\kappa}{2}k^2 + 4\pi\gamma\delta_{k,0} \tag{18.277}$$

Only the even linear combinations are physically relevant, and note that the k does in general not coincide with the excitation number n as used in the first Born-Oppenheimer equation, where the energy curves ϵ_n were sorted by energy.

The term $4\pi\gamma$ contributes only for k = 0 since all other plane waves integrate to zero in the second line of Eq. (18.256). Even when the omission of (18.276) is not valid, the integral still becomes substantial if $A_n^{(q_+)}(q_-)$ has no nodes, whereas it is suppressed when there are sign changes in $A_n^{(q_+)}(q_-)$.

In figure 18.78 we notice some discontinuities in the approximate energies, which can be explained in the following way. Due to the linear dependence of the energy for the k = 0 plane wave, its energy becomes degenerate with the higher levels, when γ varies. More precisely, $\tilde{\epsilon}_0$ will cross $\tilde{\epsilon}_k$ at the γ -value

$$\gamma_k = \frac{\kappa k^2}{8\pi} \tag{18.278}$$

Without the symmetry requirement (18.260) we could find two families of solutions to the second Born-Oppenheimer equation for each potential curve $\epsilon_n(q_+)$. Depending on the symmetries of the solution $A_n^{(q_+)}(q_-)$ discussed in *B. Energies* section earlier, we can only choose one of these families, and at each side of the energy crossing (18.278), we must discard one or the other and thus obtain a discontinuous energy dependence.

Even though figure 18.76 is obtained with moderate values of γ and κ , we see the similarity between the numerically determined $A_n^{(q_+)}(q_-)$ and plane waves, while the energy levels $\epsilon_n(q_+)$ are clearly not constant. This is due to the term (18.276), the effect of which we will approximate using non-degenerate perturbation theory. Due to the orthogonality between the cosine functions, there are no first-order corrections. The second order corrections, on the other hand, give contributions of the form

$$\Delta \tilde{\epsilon}_k(q_+) = a_k F(q_+)^2 \tag{18.279}$$

where the amplitude a_k can be calculated

$$a_{k} = \begin{cases} -\frac{1}{\kappa - 8\pi\gamma} & k = 0\\ \frac{1}{2\kappa - 16\pi\gamma} & k = \pm 1\\ \frac{1}{\kappa(4k^{2} - 1)} & \text{otherwise} \end{cases}$$
(18.280)

as shown below.

Calculation of perturbation terms

The second order perturbation terms for the potential curves $\tilde{\epsilon}_k(q_+)$ are found by calculating the matrix elements of the terms (18.276) between pairs of unperturbed eigenfunctions which are plane waves:

$$I_{l,k} \equiv -\frac{F(q_{+})}{4\pi} \int_{-2\pi}^{+2\pi} dq_{-} e^{i(k-l)q_{-}/2} \cos\left(\frac{q_{-}}{2}\right)$$
(18.281)

Using the orthogonality of the cosine functions we see that only coefficients with neighboring values of l and k are coupled

$$I_{l,k} = --\frac{F(q_{+})}{2} [\delta_{k-l+1} + \delta_{k-l-1}]$$
(18.282)

The resulting perturbative corrections then takes the form

$$\delta \tilde{\epsilon}_k(q_+) = \sum_{l \neq k}^{\infty} \frac{|I_{lk}|^2}{\tilde{\epsilon}_k - \tilde{\epsilon}_m} = a_k F(q_+)^2$$
(18.283)

where the amplitude of the oscillation is

$$a_k = \sum_{l \neq k}^{\infty} \frac{\left[\delta_{k-l+1} + \delta_{k-l-1}\right]^2}{2\kappa(k^2 - l^2) + 16\pi\gamma(\delta_{k,0} - \delta_{l,0})}$$
(18.284)

Here we can distinguish between the three cases k = 0, $k = \pm 1$ and $|k| \ge 2$, where we get the results summarized in Eq. (18.280).

This gives the perturbative approximation to the potential curves

$$\tilde{\epsilon}_{k}(q_{+}) + \delta\tilde{\epsilon}_{k}(q_{+}) = \frac{\kappa}{2}k^{2} + 4\pi\gamma\delta_{k,0} + a_{k}F(q_{+})^{2}$$
$$= \frac{\kappa}{2}k^{2} + 4\pi\gamma\delta_{k,0} + \frac{a_{k}}{2}(1 + \cos(q_{+}))$$
(18.285)

Due to the term $4\pi\gamma$ in the expression for $\tilde{\epsilon}_0(q_+)$, the energies of the eigenfunctions in this potential change linearly with γ . For $k \ge 1$ the position of $\tilde{\epsilon}_n(q_+)$ depends less strongly on γ and the eigenstates in these potentials have almost constant energy.

D. Approximate solution of the second Born-Oppenheimer equation

To analyze in more detail how the eigenenergies $E_m^{(n)}$ are distributed we must take a closer look at the second Born-Oppenheimer equation which has the form of a Schrodinger equation for a particle of mass $\hbar^2/4k$ in the potential $\epsilon_n(q_+)$. When the above perturbative treatment is valid, this potential is a cosine with amplitude $|a_k|/2$, so in order to estimate the eigenstates and energies, we must compare κ and $|a_k|$. In the limit where we can neglect the q_+ -dependence of $\tilde{\epsilon}_k(q_+)$, the solutions can be well approximated by plane waves $e^{imq_+}/\sqrt{2\pi}$ with box potential-energies

$$\tilde{E}_{m}^{(k)} = \frac{\kappa}{2}k^{2} + 4\pi\gamma\delta_{k,0} + 2\kappa m^{2}$$
(18.286)

which depend quadratically on m. In the opposite limit where $\tilde{\epsilon}_k(q_+)$ s a deep potential in (18.257), we can approximate the cosine potential by a quadratic expansion around its minimum. The resulting equation is a Schrödinger equation for a particle with mass $\hbar^2/4k$ in a harmonic oscillator of frequency

$$\omega_k = \frac{1}{\hbar} \sqrt{2\kappa |a_k|} \tag{18.287}$$

For the lower part of the energy spectrum the solutions are then well approximated by the usual harmonic oscillator eigenstate wave functions and the energies are equidistantly spaced with spacing $\hbar\omega_k$:

$$\tilde{E}_{m}^{(k)} = \left(\frac{\kappa}{2}k^{2} + 4\pi\gamma\delta_{k,0} + \frac{a_{k}}{2}\right) + \left(m + \frac{1}{2}\right)\sqrt{2\kappa|a_{k}|}$$
(18.288)

Figure 18.79 illustrates the transition between the *particle in a box* and the harmonic oscillator regimes by showing the exact and approximate energies $E_m^{(0)}$ as functions of κ for fixed negative γ . Since the harmonic oscillator approximation is valid when the potential in (18.257) is deep, it requires that $\kappa \ll |a_0| = |\kappa - 8\pi\gamma|^{-1}$, so to capture the whole transition, the κ -axis is logarithmic. The energies are plotted after subtracting the ground state energy E_0 and scaling by the energy difference $E_1 - E_0$ between the first excited state and the ground state. For $\kappa \ll 1$ the harmonic oscillator spectrum is then revealed as levels with unit spacing. For $\kappa \to 1$, on the other hand, the curves become constant at $1, 4, 9, \dots$ showing the quadratic dependence on m. We note that there is a perfect agreement between the exact and approximate energies shown in the figure. In the transition from the harmonic oscillator regime to the *particle* in a box regime the energy levels group in pairs, which has the following explanation: For a deep potential curve ϵ_n there is a significant energy difference between the first excited even and odd states, but when the potential curve is nearly constant, then even and odd solutions with a given wave number has almost the same energy. This is exemplified in the eigenfunctions in the upper panels of figure 18.76.



Figure 18.79: Exact and approximate energies as a function of κ for $\gamma = -10$. The black dashed curves show the exact energies E_n , while the solid red curves show the approximate energies $E_m^{(0)}$ found from the lowest potential-curve in the second Born-Oppenheimer equation. The green curve shows the position of the maximum of the lowest potential curve $\epsilon_0(q_+)$ within the perturbative approximation. The exact ground state energy E_0 , which varies with κ , has been subtracted from all energies, and afterward, the energies is scaled by the energy difference between the two lowest exact energy levels $E_1 - E_0$.

No matter how deep the potential curve $\tilde{\epsilon}_k(q_+)$ is, the harmonic approximation is not perfect, and above some energy the spectrum is ill-described by a harmonic oscillator spectrum. A simple estimate suggests that the description is good for eigenstates whose energies lie below the maximum of the potential curve, which is approximated by the unperturbed energies plus a term depending on the sign of a_k

$$t_k(\gamma,\kappa) = \frac{\kappa}{2}k^2 + 4\pi\gamma\delta_{k,0} + \frac{a_k + |a_k|}{2}$$
(18.289)

In figure 18.79 this (solid green) curve is shown for k = 0 and agrees systemati-

cally with the border where the harmonic oscillator energy spectrum is significantly altered.

18.7.6 Conclusions

n the present paper we have considered two identical bosons on an infinite, discrete lattice with an additional harmonic confinement. In the tight binding approximation, the single particle physics in terms of quasi- momenta is described by the same equation as a single particle in a continuous cosine potential - namely the Mathieu equation. Adding a contact interaction yields a Hamiltonian which does not separate in relative and center-of-mass coordinates, even though the two-body interaction problem separates in both a homogeneous discrete lattice Hamiltonian and in a continuous harmonic oscillator.

By formulating the problem in quasi-momentum representation we can make an approximation which is mathematically equivalent to the Born-Oppenheimer approximation performed in position space in molecular physics: We thus find approximate solutions by first solving an equation for the relative quasi-momentum wave function that depends parametrically on the center-of-mass quasi-momentum. This yields potential curves for a Schrodinger equation for the center-of-mass coordinate, which is readily solved. Contrary to the Born-Oppenheimer approximation used to separate slow nuclear and fast electronic motion in molecules, in our system we have a tunable adiabaticity parameter, namely the strength of the inter-particle interaction.

In the solution of both the first and second Born-Oppenheimer equations we can identify the excitation degrees of freedom in the system. This provides physically motivated quantum numbers valid also for the exact eigenstates together with rules for which quantum numbers are allowed by symmetry considerations.

Finally, from the good agreement between the exact and approximate solutions we conclude that the Born-Oppenheimer is well justified when the energy scales for the relative and the center-of-mass motion of the two-particle quantum state are well-separated. We imagine that a similar separation may be useful for approximate first principle calculations on many other cold atom systems, e.g., with more particles and possibly with mixtures of different species.

18.8 Spontaneous symmetry breaking in quantum mechanics

We now present a mathematically simple procedure to explain spontaneous symmetry breaking in quantum systems. The procedure is applicable to a wide range of models and can be easily used to explain the existence of a symmetry broken state in crystals, antiferromagnets, and even superconductors. It has the advantage that it automatically brings to the fore the main players in spontaneous symmetry breaking: the symmetry-breaking field, the thermodynamic limit, and the global excitations of a *thin* spectrum.

18.8.1 Introduction

In quantum mechanics symmetry has a much more powerful role than in classical mechanics. Translational invariance in a classical system causes momentum to be conserved; in quantum mechanics it immediately implies that all eigenstates of the Hamiltonian are spread out with equal amplitude over all of space. It could be argued that because a chair is built of many microscopic particles that all obey the rules of quantum mechanics, the chair as a whole should also respect the symmetry of its Hamiltonian and be spread out over all of space. Clearly this situation is not physically realized. The way out of the seeming paradox is the *spontaneous symmetry breaking* of the collective system. The description of spontaneous symmetry breaking in macroscopic systems that are constructed from microscopic, quantum mechanical constituents is one of the highlights of condensed matter theory. It is used to explain the classical features of macroscopic systems ranging from crystals and antiferromagnets to superconductors.

In this section, we present a simple mathematical procedure that can be applied to the spontaneous breaking of any continuous symmetry and that naturally emphasizes the roles of the key players (the symmetry-breaking field, the thermodynamic limit, and the global excitations of a *thin* spectrum) in this symmetry breaking. The procedure is described by considering the example of a quantum harmonic crystal that spontaneously breaks translational symmetry. All of the methods, that is, bosonization, using the Bogoliubov transformation to identify the *thin* spectrum of states involved in spontaneous symmetry breaking, introducing a symmetry-breaking field in the collective dynamics, and considering a noncommuting order of limits, can be applied to other systems as well.

18.8.2 The Harmonic Crystal

As a basic example of spontaneous symmetry breaking, we consider how translational symmetry is broken in a crystalline lattice. Consider a harmonic crystal with the Hamiltonian

$$H = \sum_{j} \frac{p_j^2}{2m} + \frac{\kappa}{2} \sum_{j} (x_j - x_{j+1})^2$$
(18.290)

where j labels the N atoms in the lattice, which have mass m, momentum p_j , and position x_j . We consider here only a one-dimensional chain of atoms, but all of the following can be straightforwardly generalized to higher dimensions. The parameter κ gives the strength of the harmonic potential between neighboring atoms. The results on spontaneous symmetry breaking that follow are equally valid for anharmonic potentials.

In the standard treatment of the harmonic oscillator a Fourier transformation of the Hamiltonian is used to identify its eigenstates. We follow a slightly longer route by introducing boson (phonon) operators from the outset and diagonalizing them using the Bogoliubov transformation discussed earlier. This approach has the advantages that it naturally brings to the fore the thin spectrum of the crystal and enables us to keep track of the center of mass motion of the crystal as a whole. The momentum and position operators can be expressed(as we have seen earlier) in terms of boson operators as

$$p_j = iC\sqrt{\frac{\hbar}{2}}(b_j^{\dagger} - b_j) \tag{18.291}$$

$$x_j = \frac{1}{C} \sqrt{\frac{\hbar}{2}} (b_j^{\dagger} + b_j) \tag{18.292}$$

so that the commutation relation $[x_j, p_{j'}] = i\hbar \delta_{j,j'}$ is satisfied.

We choose C^2 = $\sqrt{2m\kappa}$ so that the Hamiltonian reduces to

$$H = \frac{\hbar}{4} \sqrt{\frac{2\kappa}{m}} \sum_{j} [2(b_{j}^{\dagger}b_{j} + b_{j}b_{j}^{\dagger}) - (b_{j}^{\dagger} + b_{j})(b_{j+1}^{\dagger} + b_{j+1})]$$
(18.293)

After a Fourier transformation we have

$$H = \sqrt{\frac{\hbar^2 \kappa}{2m}} \sum_{k} \left[A_k b_k^{\dagger} b_k + \frac{B_k}{2} (b_k^{\dagger} b_{-k}^{\dagger} + b_k b_{-k}) + 1 \right]$$
(18.294)

where $A_k = 2 - 2\cos(ka)$, $B_k = -\cos(ka)$, and a is the lattice constant. This Hamiltonian is still not diagonal, because the terms $b_k^{\dagger}b_{-k}^{\dagger}$ and b_kb_{-k} create and annihilate two bosons at the same time. We get rid of these terms by introducing transformed operators $\beta_k = \cosh(u_k)b_{-k} + \sinh(u_k)b_k^{\dagger}$ and choosing u_k such that the resulting Hamiltonian is diagonal. After this Bogoliubov transformation, the Hamiltonian in terms of transformed bosons is given by

$$H = \hbar \sqrt{\frac{\kappa}{m}} \sum_{k} \left[2 \sin \left| \frac{ka}{2} \right| \left(\beta_{k}^{\dagger} \beta_{k} + \frac{1}{2} \right) + \frac{1}{4} \sqrt{2} \cos \left(ka \right) \right]$$
$$= 2\hbar \sqrt{\frac{\kappa}{m}} \sum_{k} \sin \left| \frac{ka}{2} \right| \left[n_{k} + \frac{1}{2} \right]$$
(18.295)

because $\sum_k \cos k = (N/2) \int_{-\pi}^{\pi} dk \cos k = 0.$

18.8.3 The Thin Spectrum

The form (18.295) of the Hamiltonian in terms of phonon operators coincides with the standard textbook results. The use of the Bogoliubov transformation to obtain Eq. (18.295) has the advantage that it draws attention to a rather subtle point. When $k \to 0$ the excitation energy $\omega_k \to 0$, and the two parameters in the Bogoliubov transformation diverge $[\sinh(u_k) \to \infty$ and $\cosh(u_k) \to \infty]$. Thus, at k = 0 the canonical transformation is no longer well defined, and we should treat the k = 0 part of the Hamiltonian (18.290) separately from the rest. The excitations with k = 0 are the ones that describe the collective dynamics of the crystal as a whole, and therefore they are also the states that are involved in the collective symmetry breaking. The k = 0 part of the Hamiltonian, written in terms of the original operators, is given by

$$H_{coll} = \frac{p_{tot}^2}{2Nm} + const.$$
(18.296)

where $p_{tot} \equiv \sum_j p_j = \sqrt{N} p_{k=0}$ is the total momentum of the system. It can easily be checked that this part of the Hamiltonian, which describes the external dynamics of the crystal as a whole, commutes with the rest of the Hamiltonian, which describes the internal dynamics of the phonon modes inside the crystal. We therefore focus on the collective part of the Hamiltonian and disregard the phonon spectrum given by Eq. (18.295).

Notice that by considering only the collective part of the Hamiltonian, we have effectively reduced the problem to a single-particle problem. The single particle in Eq. (18.296) with mass Nm and momentum p_{tot} describes the dynamics of the crystal as a whole. Its momentum and position are the center of mass momentum and position of the crystal. In contrast, Eq. (18.295) describes the internal degrees of freedom of the crystal and includes all many-body effects that arise from the coupling of the N individual atoms.

The relevant eigenstates of the collective Hamiltonian (18.296) are very low in energy: their excitation energies scale as 1/N, where N is the number of atoms in the crystal. In the thermodynamic limit all of these states thus become nearly degenerate. Because of this property a combination of these states that break the symmetry of the Hamiltonian can be spontaneously formed in the thermodynamic limit. At the same time, these collective eigenstates are so few in number and of such low energy that their contribution to the free energy completely disappears in the thermodynamic limit. This vanishing contribution can be seen by looking at their contribution to the partition function

$$Z_{thin} = \sum e^{-\beta H_{coll}} \propto \sqrt{N} \tag{18.297}$$

and the free energy

$$F_{thin} = -T \ln \left(Z_{thin} \right) \propto \ln \left(N \right) \tag{18.298}$$

The free energy of the total system is an extensive quantity, so that $F_{thin}/F_{tot} \propto \ln{(N)}/N$ disappears in the limit $N \to \infty$. The states of this part of the spectrum are thus invisible in thermodynamically measurable quantities such as for instance the specific heat of macroscopic crystals, and it is consequently called

the thin spectrum of the quantum crystal.

To see how the states in the thin spectrum can conspire to break the translational symmetry, we need to add a small symmetry-breaking field to the Hamiltonian:

$$H_{coll}^{SB} = \frac{p_{tot}^2}{2Nm} + \frac{B}{2}x_{tot}^2$$
(18.299)

Here the symmetry-breaking field B is introduced as a mathematical tool and need not actually exist. We will send the value of B to zero at the end of the calculation. The Hamiltonian (18.299) is the standard form of the Hamiltonian for a quantum harmonic oscillator, and its eigenstates are well known. The ground state wavefunction can be written as

$$\psi_0(x_{tot}) = \left(\frac{m\omega N}{\pi\hbar}\right)^{1/4} e^{-(m\omega N/2\hbar)x_{tot}^2}$$
(18.300)

with $\omega = \sqrt{B/mN}$. This ground state is a wavepacket of the total momentum states that make up the thin spectrum. Apart from the ground state configuration there are also collective eigenstates that are described by the excitations of the harmonic oscillator Eq. (18.299). These excitations describe the collective motion of the crystal as a whole. As N becomes larger, the ground state wavepacket becomes more and more localized at the position $x_{tot} = 0$, until it is completely localized as $N \to \infty$. That this localization can occur spontaneously without the existence of a physical symmetry-breaking field B can be seen by considering the noncommuting limits

$$\lim_{N \to \infty} \lim_{B \to 0} |\psi_0(x_{tot})|^2 = const.$$
(18.301)

$$\lim_{B \to 0} \lim_{N \to \infty} |\psi_0(x_{tot})|^2 = \delta(x_{tot})$$
(18.302)

If we do not include any symmetry-breaking field, then the crystal is always completely delocalized and respects the symmetry of the Hamiltonian. If we do allow for a symmetry-breaking field, then it turns out that in the limit of having infinitely many constituent particles, an infinitesimally small symmetry-breaking field is enough to completely localize the crystal at a single position. This mathematical instability implies that the symmetry breaking happens spontaneously in the thermodynamic limit.

Notice that once the crystal has been localized at a specific position and the unphysical symmetry-breaking field has been sent to zero, the delocalization of the crystal due to the spreading of its wavefunction will take a time proportional to N and can thus never be observed.

To see more rigorously whether or not the crystal as a whole is localized, we should look at the spatial fluctuations of the crystal $\langle x_{tot}^2 \rangle$. The absolute size of these fluctuations by itself is meaningless. Their size becomes meaningful

only if it is compared to the size of the crystal. Because the size of the crystal is proportional to the number of particles in the system, the appropriate order parameter in this case is $\langle x_{tot}^2 \rangle / N$. This order parameter has a noncommuting order of limits a $N \to \infty$,

$$\lim_{N \to \infty} \lim_{B \to 0} \langle x_{tot}^2 \rangle / N = \infty$$
(18.303)

$$\lim_{B \to 0} \lim_{N \to \infty} \langle x_{tot}^2 \rangle / N = 0 \tag{18.304}$$

which again signals the spontaneous localization of the crystal as a whole.

18.8.4 Subtleties

In the derivation of the spontaneous symmetry breaking of a harmonic crystal we have been somewhat sloppy in the definition of the symmetry-breaking field. After all, the collective model of Eq. (18.296) was only the k = 0 part of the full blown Hamiltonian in Eq. (18.290), but we did not consider the symmetry-breaking field to be only the k = 0 part of some other field acting on all atoms individually. It would there- fore be better to start with a microscopic model, which al- ready includes a symmetry-breaking field such as

$$H^{SB} = \sum_{j} \left[\frac{p_{j}^{2}}{2m} + \frac{\kappa}{2} (x_{j} - x_{j+1})^{2} + B(1 - \cos(x_{j})) \right]$$

$$\rightarrow H^{SB}_{coll} \simeq \frac{p_{tot}^{2}}{2Nm} + \frac{B}{2} x_{tot}^{2}$$
(18.305)

In Eq. (18.305) we again consider only the k = 0 part of the Hamiltonian and have expanded the cosine to quadratic order. The fact that the symmetrybreaking field now scales as 1/N is a direct consequence of our definition of the microscopic symmetry-breaking field. The factor 1/N cannot be avoided if we insist that the microscopic Hamiltonian be extensive. This factor might seem to imply an end to the localization of the total wavefunction $\psi_0(x_{tot})$, but spontaneous symmetry breaking is still possible as long as we con-sider the correct order parameter. Even though the wavefunction itself does not reduce to a Dirac delta function anymore, the spatial fluctuations of the crystal compared to its size still become negligible in the thermodynamic limit if an infinitesimal symmetry-breaking field is included:

$$\lim_{N \to \infty} \lim_{B \to 0} \langle x_{tot}^2 \rangle / N = \infty$$
 (18.306)

$$\lim_{B \to 0} \lim_{N \to \infty} \langle x_{tot}^2 \rangle / N = 0$$
(18.307)

Once again the disappearance of fluctuations in the thermo- dynamic limit signals the spontaneous localization of the crystal as a whole.

This digression into extensivity and the correct choice for the symmetry-breaking

field seems unnecessary for understanding the essential ingredients of spontaneous symmetry breaking, and therefore we have ignored these subtleties in our main treatment of quantum spontaneous symmetry breaking. In the application of this procedure to other systems, such as antiferromagnets and superconductors, these issues don't arise because we are forced to consider extensive models from the outset. In these cases, however, the mathematics of diagonalizing the collective Hamiltonian is a bit more involved.

18.8.5 Discussion

We have presented a simple way of explaining the appearance of spontaneous symmetry breaking in quantum systems. The procedure starts with the bosonization of the microscopic Hamiltonian. The quadratic part of the bosonized Hamiltonian can in principle be diagonalized using a Bogoliubov transformation, but in doing so we find that there are some modes for which the transformation is ill-defined. These singular modes are the ones that describe the dynamics of the system as a whole (in contrast to the dynamics of constituent particles within the system). These collective excitations should be treated separately from all other modes, and together they define the collective part of the Hamiltonian of the system. The eigenstates of this collective Hamiltonian that scale as 1/Nform the thin spectrum. It is a combination of these states that make up the symmetry broken wavefunction. As a mathematical tool necessary to be able to see the symmetry breaking explicitly, we introduced the symmetry-breaking field B. If we look at the new ground state wavefunction or at a suitably defined order parameter for the system, we see that in the thermodynamic limit an infinitesimally small field B is enough to completely break the symmetry of the underlying Hamiltonian. It is thus argued that symmetry breaking can happen spontaneously in the limit $N \to \infty$.

The method as presented here can be adapted to describe rotors, antiferromagnets, and even superconductors, and should in principle be applicable to all quantum systems that spontaneously break some continuous symmetry.

18.9 Problems

18.9.1 Piecewise Constant Potential Energy One Atom per Primitive Cell

Consider a one-dimensional crystal whose potential energy is a piecewise constant function of x. Assume that there is one atom per primitive unit cell - that is, we are using the Kronig-Penney model as shown below.

(a) Let s = d/2 (same spacing as in the text) and explain why no energy gap occurs at the second Brillouin zone boundary in the weak-binding limit, using physical argument based on sketches of the electron probability density.



Figure 18.80: Piecewise Constant Potential - 1 Atom per Primitive Cell

(b) For s = d/3, what are the magnitudes of the lowest six band gaps in the weak binding limit?

18.9.2 Piecewise Constant Potential Energy Two Atoms per Primitive Cell

Consider a one-dimensional crystal with two atoms per primitive unit cell as shown below.



Figure 18.81: Piecewise Constant Potential - 2 Atoms per Primitive Cell

- (a) Using the weak-binding approximation, determine the band gap for an arbitrary Brillouin zone boundary.
- (b) Use the results of part (a) to obtain an expression for the band gaps for $w \ll d$ and zone boundaries corresponding to small values of G. Are any of these band gaps zero? Use physical arguments to explain why or why not.
- (c) Use the results of part(a) to determine the magnitude of the lowest eight band gaps for w = d/4. Are any of these band gaps zero? Use physical arguments to explain why or why not.
- (d) In the weak-binding approximation, the energies for wave vectors k that are far from the Brillouin zone boundaries are given by the free-electron

energies $E = \hbar^2 k^2/2m_e$. In relation to the zero of V(x) above, from what value of the energy are the free-electron energies measured? Does any-thing unusual happen when the energies exceed zero - the beginning of the continuum for the isolated atoms? Determine how many band gaps occur below E = 0. Answer these questions using the weak-binding approximation.

18.9.3 Free-Electron Energy Bands for a Crystal with a Primitive Rectangular Bravais Lattice

Consider a two-dimensional crystal with a primitive rectangular Bravais lattice. Take the ratio of sides of the rectangular primitive cell to be 2:1, where the larger side is along the y-axis.

(a) Working in the reduced zone scheme, sketch the free-electron energy for the four lowest bands as a function of the distance in \vec{k} space (starting at $\vec{k} = 0$) along the path in the first Brillouin zone shown in the figure below.



Figure 18.82: Paths in the First Brillouin Zone

- (b) Sketch free-electron constant energy contours in the reduced zone scheme for the lowest four bands.
- (c) Sketch the free-electron density of states, $\mathcal{D}^{(n)}(E)$, for each of the four lowest bands individually. Sketch $\mathcal{D}(E)$ for the total of the four lowest bands.
- (d) Sketch the free-electron Fermi surfaces in the reduced zone scheme for $\eta = 1 \ to \ 6$. Indicate the positions of the various Fermi energies on the density-of-states graphs of part (c). Use quantitatively correct values for k_F and E_F in this part.

18.9.4 Weak-Binding Energy Bands for a Crystal with a Hexagonal Bravais Lattice

Consider a two-dimensional crystal with an hexagonal rectangular Bravais lattice oriented so that two nearest lattice points can lie along the y-axis but not
along the x-axis.

(a) Using the reduced zone scheme, sketch the energy versus distance in \bar{k} space (starting at $\bar{k} = 0$) along the path in the first Brillouin zone shown in the figure below. Do this for the six lowest bands in both the freeelectron and weak-binding approximations (assuming (incorrectly) that all degeneracies are absent in the latter case).



Figure 18.83: Paths in the First Brillouin Zone

- (b) Sketch constant energy contours in the reduced zone scheme for the lowest six bands. Do so in both the free-electron and weak-binding approximations. Indicate the location in \vec{k} space of all distinct maxima, minima and saddlepoints (only one of a set that are equivalent by symmetry need be shown).
- (c) Sketch the Fermi *surface* in the reduced zone scheme for $\eta = 1 \text{ to } 7$. Do so in both the free-electron and weak-binding approximations. Use quantitatively correct values for k_F in the free-electron sketches.
- (d) Sketch the density of states, $\mathcal{D}^{(n)}(E)$, for each of the five lowest bands individually and $\mathcal{D}(E)$ for the total of the five lowest bands. Do so in both the free-electron and weak-binding approximations. Assume all degeneracies are absent in the latter case and make reasonable assumptions about the sense of the energy shifts from the free-electron values at the singular points.
- (e) For which integral value of η would insulating properties be most likely to first occur as the strength of the periodic potential energy is increased? Why?

18.9.5 A Weak-Binding Calculation #1

Consider a two-dimensional crystal with a primitive rectangular Bravais lattice and two identical atoms per primitive unit cell. Take the structure to be as shown below with a:b:c::4:2:1. Take the potential energy to be the sum of the potential energies for the individual atoms located at the atom sites given in the figure. Use the weak-binding approximation.



Figure 18.84: 2-Dimensional Crystal - Rectangular Bravais Lattice with 2 Atoms per Primitive Unit Cell

- (a) Find expressions for the matrix elements V_G that describe the band gaps in the weak-binding limit. Under what circumstances, if any, is $V_G = 0$?
- (b) Use the results of part (a) to draw qualitatively correct constant energy contours in the reduced zone scheme for the lowest three bands.
- (c) Sketch qualitatively correct individual band densities of states for the lowest three bands.

18.9.6 Weak-Binding Calculations with Delta-Function Potential Energies

Consider a two-dimensional crystal for which the potential energy consists of delta functions, one for each atom. Use the weak-binding approximation .

- (a) For the case of one atom per primitive cell, obtain a general expression for the energy difference between adjacent bands at a Brillouin zone boundary where they would be degenerate in the free-electron approximation (ignoring the intersections of two or more boundaries). How does this result depend on the Bravais lattice (assuming the area of a primitive cell is the same for each different case)?
- (b) For a crystal with a square lattice and one atom per primitive unit cell, what are the energies of the lowest four bands at $\vec{k} = (\pi/d)(1,1)$? Explain your result in a physical and qualitative way.
- (c) For a crystal with a centered rectangular Bravais lattice and two different delta-function atoms per primitive unit cell as shown in the figure below, evaluate the energy splittings between the bands for all zone boundaries in the extended zone scheme for the five lowest bands (ignore all intersections of two or more boundaries).



Figure 18.85: 2-Dimensional Crystal - Centered Rectangular Bravais Lattice with 2 Atoms per Primitive Unit Cell

18.9.7 Is the spectrum of the harmonic crystal example really *thin*?

Check that the thin spectrum of a harmonic crystal is indeed thin. That is,

- (a) Show that only the lowest \sqrt{N} total momentum states are not exponentially suppressed in the symmetry broken wavefunction (18.300). (This result implies that only the lowest \sqrt{N} total momentum states contribute to the symmetry broken wavefunction, and these states all be-come degenerate in the thermodynamic limit).
- (b) Calculate the partition function of the thin spectrum states and show that it scales as \sqrt{N} , so that the contribution of these states to the free energy vanishes in the thermodynamic limit.

18.9.8 Are the limits really noncommutative in the harmonic crystal example?

Show the noncommutativity of the limits in Eq. (18.304) explicitly, by going through the following steps:

- (a) Formulate the Hamiltonian of Eq. (18.299) in terms of the boson (raising and lowering) operators $b^{\dagger} = \sqrt{C/(2\hbar)}(x_{tot} (i/C)p_{tot})$ and $b = \sqrt{C/(2\hbar)}(x_{tot} + (i/C)p_{tot})$ (where C is some constant).
- (b) Choose C such that the Hamiltonian becomes diagonal and find its ground state.
- (c) Evaluate the limits of Eq. (18.304) by expressing x_{tot}^2 in terms of boson operators and taking the expectation value with respect to the ground state of H_{coll}^{SB} .

18.9.9 The Bogoliubov transformation in the harmonic crystal example.

Work out the Bogoliubov transformation of Eqs. (18.294) and (18.295) explicitly.

- (a) Write the Hamiltonian of Eq. (18.294) in terms of the trans- formed bosons $\beta_k = \cosh(u_k)b_{-k} + \sinh(u_k)b_k^{\dagger}$.
- (b) Which value should be chosen for u_k in order for the Bogoliubov transformation to yield the diagonal Hamiltonian of Eq. (18.295)? [Answer: $\tanh(2u_k) = B_k/A_k$]

Chapter 19

Second Quantization

19.1 Identical Particles Revisited

When dealing with a system that contains only a few identical particles, we were easily able to explicitly construct appropriately symmetrized state vectors. However, when the number of identical particles in the system gets very large as with electrons in a metal, superfluids or superconductors and so on, these methods become too cumbersome to use effectively.

To see how to proceed in these cases, we will step back, revisit the subject of identical particles and look for an alternative way of thinking about such systems.

19.1.1 Indistinguishability

As we saw earlier, in quantum mechanics, the state of a system with identical particles can be described by a set of quantum numbers corresponding to the eigenvalues of a commuting set of single-particle operators representing singleparticle observables.

When we specify a state vector we designate how many particles have certain sets of quantum numbers, i.e.,

 n_1 particles have quantum number set K_1 n_2 particles have quantum number set K_2 and so on

More complicated states are then superpositions of these states.

The important fact is that, for identical or indistinguishable particles, it is impossible to state which particle has K_1 , which particle has K_2 , etc. As we saw in atoms, this indistinguishability has measurable effects on energy levels arising from particle exchange symmetries.

19.1.2 State Vectors

When we define a state vector for a system of n identical particles we are working under the following assumption

any complete set of quantum numbers (observables) that can be used to describe the behavior of a single particle can also be used for n non-interacting particles of the same type

This assumption is postulated to be true even if the n particles are interacting. The assumption implies that *composite systems* somehow *retain* the information *related* to single-particle properties.

Mathematically it says that

for each set of quantum numbers K_i there exists an *occupation* number operator \hat{N}_i such that the eigenvectors of \hat{N}_i imply states in which a definite number, n_i , of particles has the quantum numbers K_i and that the eigenvalues of the \hat{N}_i are the occupation numbers n_i .

We make the fundamental *postulate* that the set of all \hat{N}_i forms a complete set of commuting Hermitian operators for any system of identical particles.

We now construct the state vector space appropriate for the many particle system by generalizing one-particle quantum mechanics and building in indistinguishability from the start.

Our postulates imply that the state vector space for the many particle system (called Fock space) has the basis vectors

$$|n_1, n_2, n_3, \dots \rangle \tag{19.1}$$

where the notation implies that

 n_1 particles have quantum number set K_1 n_2 particles have quantum number set K_2 and so on

As we said, we assume this set is a complete orthonormal basis.

In this vector space, we define

$$|0\rangle = |0, 0, 0, 0, \dots \rangle$$
 = zero particle or vacuum state (19.2)

and one-particle states are of the form

$$|0, 0, 0, \dots, 0, n_i = 1, 0, 0, \dots \rangle$$
 (19.3)

These one-particle states span the one-particle subspace of the much larger state space of the many particle system.

Most of the quantum mechanics we have developed so far applies to these oneparticle states.

We now ask whether the postulate implies enough formalism to construct a quantum mechanics of a many-particle interacting system?

To answer this question **yes**, we must show that a consistent framework exists that makes predictions in agreement with experiment.

The fundamental assumption that the states of an interacting system can be written in terms of states for noninteracting single particles comes from our experience with perturbation theory. It will fail to work if the noninteracting and interacting states are two *inequivalent* representations of the Hilbert space for the many particle system. Standard perturbation theory implicitly assumes that the zero-order or unperturbed states and the exact states are equivalent representations of the Hilbert space.

19.2 Occupation Number Space

19.2.1 Creation and Annihilation Operators

Earlier we studied the \hat{a} , \hat{a}^+ operators in conjunction with the harmonic oscillator problem. In that system we found that \hat{a} lowered the energy of the system by 1 quantum = $\hbar\omega$, while \hat{a}^+ raised the energy of the system by $\hbar\omega$.

In terms of the eigenvalues and eigenvectors of the number operator $\hat{N} = \hat{a}^+ \hat{a}$ where $\hat{N} |n\rangle = n |n\rangle$ we found that

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$
 and $\hat{a}^{+}|n\rangle = \sqrt{n+1}|n+1\rangle$ (19.4)

In some sense, we can think of the \hat{a} , \hat{a}^+ as annihilation/creation operators for a quantum of the energy associated with a single particle system.

Another appearance of operators of this type with similar properties will occur when we study the interaction of radiation with matter in Chapter 20. We will be able to introduce photon annihilation/creation operators which remove/add a single photon with particular quantum numbers $(\vec{k}, \vec{\lambda})$ corresponding to photon momentum and polarization. The photon operators will have same mathematical structure(commutators) as the \hat{a} , \hat{a}^+ operators of the harmonic oscillator system.

In the photon case, as we will see, the states of the system will be the photon number states given by

$$|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, N_{\vec{k}_3\vec{\lambda}_3}, \dots \rangle$$
(19.5)

We will base our generalization on these examples. The generalization will allow us eventually to define the most general Fock space for any many particle system.

Suppose that we have a potential well $V(\vec{r})$ with single particle energy eigenstates given by

$$\phi_0(\vec{r}) = \langle \vec{r} \mid 0 \rangle \quad , \quad \phi_1(\vec{r}) = \langle \vec{r} \mid 1 \rangle \quad , \quad \phi_2(\vec{r}) = \langle \vec{r} \mid 2 \rangle \quad , \dots \dots \dots \quad (19.6)$$

We start the discussion by considering a system of n bosons.

We assume that all n particles are in the lowest level (ground state) $\phi_0(\vec{r})$ of the well. We label this state by the symbol $|n\rangle$ where $n = 0, 1, 2, 3, \dots$, i.e., $|0\rangle$ is the state with no particles in the lowest level.

We now introduce the operators \hat{a}_0 , \hat{a}_0^+ such that

$$\hat{a}_0 |n\rangle = \sqrt{n} |n-1\rangle \quad and \quad \hat{a}_0^+ |n\rangle = \sqrt{n+1} |n+1\rangle \tag{19.7}$$

By definition, these operators relate states of the *n*-boson system with all *n* particles in $\phi_0(\vec{r})$ to those states of an $n \pm 1$ particle system with all particles in $\phi_0(\vec{r})$. In this sense, we say that

 $\hat{a}_0 =$ a particle annihilation operator

which removes a particle in the state $\phi_0(\vec{r})$ from the system

 \hat{a}_0^+ = a particle creation operator

which adds a particle in the state $\phi_0(\vec{r})$ to the system

These operators, by construction, have the same algebra as the harmonic oscillator operators, i.e.,

$$[\hat{a}_0, \hat{a}_0^+] = 1$$
 , $[\hat{a}_0, \hat{a}_0] = 0 = [\hat{a}_0^+, \hat{a}_0^+]$ (19.8)

and

$$|n\rangle = \frac{\left(\hat{a}_{0}^{+}\right)^{n}}{\sqrt{n!}}|0\rangle \quad , \quad \hat{a}_{0}|0\rangle = 0 \quad (\text{no particles to be annihilated})$$
(19.9)

This says that

the state with n particles in the lowest level, $|n\rangle$, is generated by *adding* n particles, in $\phi_0(\vec{r})$, to the *vacuum* state $|0\rangle$

Acting to the left (instead of to the right) these operators reverse their roles, i.e.,

$$\langle n | \hat{a}_0 = \sqrt{n+1} \langle n+1 | \rightarrow \text{ adds particles in the state } \phi_0(\vec{r})$$

 $\langle n | \hat{a}_0^+ = \sqrt{n} \langle n-1 | \rightarrow \text{ removes particles in the state } \phi_0(\vec{r})$

The operator

$$\hat{N}_0 = \hat{a}_0^+ \hat{a}_0 \tag{19.10}$$

measures the number of particles in a state since

$$\hat{N}_0 \left| n \right\rangle = \hat{a}_0^+ \hat{a}_0 \left| n \right\rangle = n \left| n \right\rangle \tag{19.11}$$

This is a very appealing picture, but really all we have done is rewrite the harmonic oscillator story using a lot of new words. We do not have any new physics yet!

Before introducing the new physical ideas, we carry out this same discussion for fermions.

In this case, the only allowed states are

$$|0\rangle =$$
no particles in $\phi_0(\vec{r})$
 $|1\rangle = 1$ particle in $\phi_0(\vec{r})$

since we cannot, according to the PEP, have two particles with the *same* quantum numbers (in the same state).

We can still introduce annihilation/creation operators but they must have a very different algebra. We must have

| $\hat{a}_0 \left 0 \right\rangle = 0$ | there are no particles to be annihilated |
|---|---|
| $\hat{a}_0 \left 1 \right\rangle = \left 0 \right\rangle$ | we can remove a particle when there is a particle |
| $\hat{a}_{0}^{+}\left 0\right\rangle =\left 1\right\rangle$ | we can add a particle when there are no particles |
| $\hat{a}_{0}^{+}\left 1\right\rangle=0$ | we cannot have two particles in the same state |

The last relation is necessary to satisfy the PEP.

We can figure out the operator algebra by using a special representation of these states and operators. We let the two states (only allowed states) be a basis and select the 2-dimensional representation

$$|0\rangle = \begin{pmatrix} 1\\0 \end{pmatrix} \quad and \quad |1\rangle = \begin{pmatrix} 0\\1 \end{pmatrix} \tag{19.12}$$

In this representation we have

$$\begin{array}{l} \left\langle 0 \right| \hat{a}_{0} \left| 0 \right\rangle = 0 \ , \ \left\langle 1 \right| \hat{a}_{0} \left| 0 \right\rangle = 0 \ , \ \left\langle 0 \right| \hat{a}_{0} \left| 1 \right\rangle = 1 \ , \ \left\langle 1 \right| \hat{a}_{0} \left| 1 \right\rangle = 0 \\ \\ \hat{a}_{0} = \left(\begin{array}{c} 0 & 1 \\ 0 & 0 \end{array} \right) \\ \left\langle 0 \right| \hat{a}_{0}^{+} \left| 0 \right\rangle = 0 \ , \ \left\langle 1 \right| \hat{a}_{0}^{+} \left| 0 \right\rangle = 1 \ , \ \left\langle 0 \right| \hat{a}_{0}^{+} \left| 1 \right\rangle = 0 \ , \ \left\langle 1 \right| \hat{a}_{0}^{+} \left| 1 \right\rangle = 0 \\ \\ \hat{a}_{0}^{+} = \left(\begin{array}{c} 0 & 0 \\ 1 & 0 \end{array} \right) \end{array}$$

Another way of representing these operators is via outer products, i.e.,

$$\hat{a}_0 = |0\rangle \langle 1| \quad , \quad \hat{a}_0^+ = |1\rangle \langle 0|$$
 (19.13)

The operator algebra is then given by

$$\hat{a}_0 \hat{a}_0^+ = |0\rangle \langle 0| = \text{ projection operator on the } |0\rangle \text{ state} \hat{a}_0^+ \hat{a}_0 = |1\rangle \langle 1| = \text{ projection operator on the } |1\rangle \text{ state} \hat{a}_0 \hat{a}_0^+ + \hat{a}_0^+ \hat{a}_0 = |0\rangle \langle 0| + |1\rangle \langle 1| = \hat{I}$$

This last relation was derived, in general, earlier and is just the sum over all projection operators.

Therefore we get

$$\{\hat{a}_0, \hat{a}_0^+\} = \hat{a}_0 \hat{a}_0^+ + \hat{a}_0^+ \hat{a}_0 = \hat{I}$$
(19.14)

Thus, the algebra involves *anticommutators* instead of commutators. That is the only change we need to make!!

We also have

$$\{\hat{a}_0, \hat{a}_0\} = 0 = \{\hat{a}_0^+, \hat{a}_0^+\}$$
(19.15)

These anticommutators imply that

 $(\hat{a}_0)^2 = 0 \rightarrow$ we cannot remove two fermions from the same state (maximum of one allowed)

 $(\hat{a}_0^+)^2 = 0 \rightarrow$ we cannot put fermions into the same state (maximum of one allowed)

Summary:

For one single particle level in a potential well, we can define annihilation/creation operators such that:

bosons have

$$[\hat{a}_0, \hat{a}_0^+] = \hat{I}$$
, $[\hat{a}_0, \hat{a}_0] = 0 = [\hat{a}_0^+, \hat{a}_0^+]$ (19.16)

and

fermions have

$$\{\hat{a}_0, \hat{a}_0^+\} = \hat{I}$$
 , $\{\hat{a}_0, \hat{a}_0\} = 0 = \{\hat{a}_0^+, \hat{a}_0^+\}$ (19.17)

We now expand our view and consider the case where particles can occupy two levels of the potential well, say $\phi_0(\vec{r})$ and $\phi_1(\vec{r})$.

For bosons, we write the state of a many particle system as

$$|n_0, n_1\rangle \tag{19.18}$$

which implies

$$n_0$$
 particles in $\phi_0(\vec{r})$ and n_1 particles in $\phi_1(\vec{r})$ (19.19)

We now define a pair of boson annihilation/creation operators by the relations

$$\hat{a}_0 |n_0, n_1\rangle = \sqrt{n_0} |n_0 - 1, n_1\rangle
\hat{a}_0^+ |n_0, n_1\rangle = \sqrt{n_0 + 1} |n_0 + 1, n_1\rangle
\hat{a}_1 |n_0, n_1\rangle = \sqrt{n_1} |n_0, n_1 - 1\rangle
\hat{a}_1^+ |n_0, n_1\rangle = \sqrt{n_1 + 1} |n_0, n_1 + 1\rangle$$

which imply that

$$\hat{a}_0$$
 annihilates a particle in the state $\phi_0(\vec{r})$

- \hat{a}_0^+ creates a particle in the state $\phi_0(\vec{r})$
- \hat{a}_1 annihilates a particle in the state $\phi_1(\vec{r})$
- \hat{a}_1^+ creates a particle in the state $\phi_1(\vec{r})$

In the same manner as in the one level case, we must have the commutator algebra

$$[\hat{a}_0, \hat{a}_0^+] = 1$$
 , $[\hat{a}_0, \hat{a}_0] = 0 = [\hat{a}_0^+, \hat{a}_0^+]$ (19.20)

and

$$[\hat{a}_1, \hat{a}_1^+] = 1$$
 , $[\hat{a}_1, \hat{a}_1] = 0 = [\hat{a}_1^+, \hat{a}_1^+]$ (19.21)

For bosons, the order in which we create or annihilate particles in a state does not matter, i.e.,

$$\hat{a}_0 \hat{a}_1 | n_0, n_1 \rangle = \hat{a}_1 \hat{a}_0 | n_0, n_1 \rangle \tag{19.22}$$

which says

$$[\hat{a}_0, \hat{a}_1] = 0 \tag{19.23}$$

In a similar way all the other mixed commutators are also zero

$$[\hat{a}_0, \hat{a}_1^+] = 0 = [\hat{a}_1, \hat{a}_0^+] = [\hat{a}_1^+, \hat{a}_0^+]$$
(19.24)

All allowed states can be constructed from the vacuum state $|0,0\rangle$ by using

$$|n_0, n_1\rangle = \frac{(\hat{a}_1^+)^{n_1}}{\sqrt{n_1!}} \frac{(\hat{a}_0^+)^{n_0}}{\sqrt{n_0!}} |0, 0\rangle$$
(19.25)

Finally,

$$\begin{split} \hat{N}_0 &= \hat{a}_0^+ \hat{a}_0 \to \quad \text{the number of particles in state} \quad \phi_0(\vec{r}) \\ \hat{N}_1 &= \hat{a}_1^+ \hat{a}_1 \to \quad \text{the number of particles in state} \quad \phi_1(\vec{r}) \end{split}$$

and

$$\hat{N} = \hat{N}_0 + \hat{N}_1 \rightarrow$$
 the total particle number operator (19.26)

Therefore,

.

$$\begin{split} \bar{N}_{0} & |n_{0}, n_{1} \rangle = n_{0} & |n_{0}, n_{1} \rangle \\ \bar{N}_{1} & |n_{0}, n_{1} \rangle = n_{1} & |n_{0}, n_{1} \rangle \\ \bar{N} & |n_{0}, n_{1} \rangle = (n_{0} + n_{1}) & |n_{0}, n_{1} \rangle \end{split}$$

Thus, for bosons we are able to just glue two single level many particle systems together to create a two-level many particle system. We are really constructing direct product states.

For fermions, however, there are some extra complications that we have to deal with.

We start off by following a similar procedure. For the two-level system we have only four possible fermion states, namely,

$$|0,0\rangle, |0,1\rangle, |1,0\rangle, |1,1\rangle$$
 (19.27)

We are *completely free* to define one set of creation/annihilation operators.

We define the \hat{a}_1 , \hat{a}_1^+ by

$$\begin{array}{ll} \hat{a}_{1} \; |0,0\rangle = 0 & , & \hat{a}_{1} \; |1,0\rangle = 0 \\ \hat{a}_{1} \; |0,1\rangle = |0,0\rangle & , & \hat{a}_{1} \; |1,1\rangle = |1,0\rangle \\ \hat{a}_{1}^{+} \; |0,0\rangle = \; |0,1\rangle & , & \hat{a}_{1}^{+} \; |1,0\rangle = \; |1,1\rangle \\ \hat{a}_{1}^{+} \; |0,1\rangle = 0 & , & \hat{a}_{1}^{+} \; |1,1\rangle = 0 \end{array}$$

For \hat{a}_0 , \hat{a}_0^+ we can freely define the operation on state with no particles in level $\phi_1(\vec{r})$

$$\hat{a}_{0} |0,0\rangle = 0 , \quad \hat{a}_{0} |1,0\rangle = |0,0\rangle \hat{a}_{0}^{+} |0,0\rangle = |1,0\rangle , \quad \hat{a}_{0}^{+} |1,0\rangle = 0$$

We must take care, however, in the fermion case when a particle exists in level $\phi_1(\vec{r})$, i.e., for the operations

$$\hat{a}_{0} |0,1\rangle$$
 , $\hat{a}_{0} |1,1\rangle$
 $\hat{a}_{0}^{+} |0,1\rangle$, $\hat{a}_{0}^{+} |1,1\rangle$

The reason we must worry about these cases is connected with our earlier discussion of a totally antisymmetric state vector for fermions, i.e., if we interchange any two identical fermions we must get a minus sign.

In this formalism, how do we interchange two fermions in the state $|1,1\rangle$? Using only the defined relations we have.....

- Step 1: $|1,1\rangle \rightarrow |1,0\rangle = \hat{a}_1 |1,1\rangle \rightarrow$ remove a particle from state $\phi_1(\vec{r})$ using \hat{a}_1
- Step 2: $|1,0\rangle \rightarrow |0,1\rangle = \hat{a}_1^+ \hat{a}_0 |1,0\rangle \rightarrow \text{transfer the particle from state } \phi_0(\vec{r}) \text{ to } \phi_1(\vec{r})$ by applying $\hat{a}_1^+ \hat{a}_0 \ (\hat{a}_0 \text{ followed by } \hat{a}_1)$
- Step 3: put the leftover particle back into $\phi_0(\vec{r})$ using \hat{a}_0^+ which gives the state relationship

$$\hat{a}_{0}^{+}\hat{a}_{1}^{+}\hat{a}_{0}\hat{a}_{1}\left|1,1\right\rangle = \hat{a}_{0}^{+}\left|0,1\right\rangle \tag{19.28}$$

However, all we have done is switch the particles in the original state $|1,1\rangle$, which means that a minus sign must appear or

$$\hat{a}_{0}^{+}|0,1\rangle = -|1,1\rangle \tag{19.29}$$

In this way, the state is completely antisymmetric under particle exchange.

In a similar manner, the other relations that complete the definition of the annihilation and creation operators are

$$\hat{a}_0 |1,1\rangle = -|0,1\rangle$$
 , $\hat{a}_0 |0,1\rangle = 0 = \hat{a}_0^+ |1,1\rangle$ (19.30)

Since $\hat{a}_0 = (\hat{a}_0^+)^+$ we have

$$\hat{a}_{0}^{+}|0,1\rangle = -|1,1\rangle$$
 , $\hat{a}_{0}\hat{a}_{0}^{+}|0,1\rangle = -\hat{a}_{0}|1,1\rangle = |0,1\rangle$ (19.31)

so that \hat{a}_0 completely undoes the operation of \hat{a}_0^+ .

These definitions, which are now consistent with complete antisymmetry correspond to the anticommutation relations

$$\begin{cases} \hat{a}_0, \hat{a}_0^+ \} = 1 & \{\hat{a}_0, \hat{a}_0\} = 0 & \{\hat{a}_0^+, \hat{a}_0^+\} = 0 \\ \{\hat{a}_1, \hat{a}_1^+ \} = 1 & \{\hat{a}_1, \hat{a}_1\} = 0 & \{\hat{a}_1^+, \hat{a}_1^+ \} = 0 \\ \{\hat{a}_0, \hat{a}_1\} = 0 & \{\hat{a}_0, \hat{a}_1^+ \} = 0 & \{\hat{a}_0^+, \hat{a}_1\} = 0 \\ \{\hat{a}_0^+, \hat{a}_1^+ \} = 0 & \end{cases}$$

We get anticommutators instead of commutators because of the complete antisymmetry under particle interchange(see argument below).

The rule for constructing the allowed states is

$$|n_0, n_1\rangle = (\hat{a}_1^+)^{n_1} (\hat{a}_0^+)^{n_0} |0, 0\rangle$$
(19.32)

Note the order, \hat{a}_0^+ acts first and we have no factorial factors since 0! = 1! = 1.

The connection between the minus sign and the anticommutators is now clear, i.e.,

$$\hat{a}_0 |1,1\rangle = \hat{a}_0 \hat{a}_1^+ \hat{a}_0^+ |0,0\rangle = -\hat{a}_1^+ \hat{a}_0 \hat{a}_0^+ |0,0\rangle$$

= $-\hat{a}_1^+ [1 - \hat{a}_0^+ \hat{a}_0] |0,0\rangle = -\hat{a}_1^+ |0,0\rangle$
= $-|0,1\rangle$

So we could have assumed the anticommutators and derived the state operations instead of going the other way.

The generalization to the many particle system where particles can occupy all of the levels is now straightforward.

In generalizing, we will not only let the particles occupy all of the levels, but also have all spin orientations.

Once again the states will be labeled

$$|n_0, n_1, n_2, \dots \rangle$$
 (19.33)

where now

 n_i = the number of particles in $\phi_i(\mathbf{r})$ with a given spin orientation (if the particles have spin)

We define creation and annihilation operators \hat{a}_i^+ and \hat{a}_i for each different single particle state.

For boson operators we have commutation relations

$$\left[\hat{a}_{i}, \hat{a}_{j}^{+}\right] = \delta_{ij} \quad , \quad \left[\hat{a}_{i}, \hat{a}_{j}\right] = 0 = \left[\hat{a}_{i}^{+}, \hat{a}_{j}^{+}\right]$$
(19.34)

and

$$|n_0, n_1, n_2, \dots\rangle = \dots \dots \frac{(\hat{a}_2^+)^{n_2}}{\sqrt{n_2!}} \frac{(\hat{a}_1^+)^{n_1}}{\sqrt{n_1!}} \frac{(\hat{a}_0^+)^{n_0}}{\sqrt{n_0!}} |0\rangle$$
(19.35)

where

$$|0\rangle = |0, 0, 0, 0, \dots \rangle$$
 = the vacuum state (19.36)

To within numerical factors, as we will see, these are the same relations we will find in Chapter 20 for photons. Therefore, *photons must be bosons* !!

For fermion operators we have anticommutation relations

$$\{\hat{a}_i, \hat{a}_j^+\} = \delta_{ij}$$
, $\{\hat{a}_i, \hat{a}_j\} = 0$, $\{\hat{a}_i^+, \hat{a}_j^+\} = 0$ (19.37)

and

$$|n_0, n_1, n_2,\rangle =(\hat{a}_2^+)^{n_2} (\hat{a}_1^+)^{n_1} (\hat{a}_0^+)^{n_0} |0\rangle$$
, $n_i = 0, 1$ only (19.38)

In both cases

$$\hat{N} = \sum_{i} \hat{N}_{i} = \sum_{i} \hat{a}_{i}^{+} a_{i}$$
(19.39)

and

$$\left[\hat{N}_i, \hat{N}_j\right] = 0 \tag{19.40}$$

19.2.2 An Example

We now consider the complete set of plane wave states in a box using periodic boundary conditions. We have -2

$$\hat{H} = \frac{\vec{p}_{op}^2}{2m}$$
(19.41)

Since

$$\left[\hat{H}, \vec{p}_{op}\right] = 0 \tag{19.42}$$

we have a common eigenbasis that we will label by $|\vec{p}\rangle$. We then have

$$\vec{p}_{op} \left| \vec{p} \right\rangle = \vec{p} \left| \vec{p} \right\rangle \quad , \quad \hat{H} \left| \vec{p} \right\rangle = \frac{\vec{p}^2}{2m} \left| \vec{p} \right\rangle = E \left| \vec{p} \right\rangle$$
(19.43)

so that

$$E = \frac{\vec{p}^2}{2m} \tag{19.44}$$

The corresponding wave functions are

$$\phi_{\vec{p}}(\vec{r}) = \langle \vec{r} \mid \vec{p} \rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}$$
(19.45)

where $\vec{p} = \hbar \vec{k}$ and V = volume of the box. The factor $1/\sqrt{V}$ normalizes the wavefunction in the box.

Periodic boundary conditions are imposed by the relations

$$\begin{split} \phi_{\vec{p}}(0,y,z) &= \phi_{\vec{p}}(L_x,y,z) \\ \phi_{\vec{p}}(x,0,z) &= \phi_{\vec{p}}(x,L_y,z) \\ \phi_{\vec{p}}(x,y,0) &= \phi_{\vec{p}}(x,y,L_z) \end{split}$$

which imply that

$$e^{ik_x L_x} = 1 \to k_x = \frac{2\pi n_x}{L_x} \quad , \quad n_x = 0, \pm 1, \pm 2, \dots$$
$$e^{ik_y L_y} = 1 \to k_y = \frac{2\pi n_y}{L_y} \quad , \quad n_y = 0, \pm 1, \pm 2, \dots$$
$$e^{ik_z L_z} = 1 \to k_z = \frac{2\pi n_z}{L_z} \quad , \quad n_z = 0, \pm 1, \pm 2, \dots$$

We now define

 $\hat{a}^+_{\vec{p}s}$ = the operator that creates (adds) a particle of momentum \vec{p} and spin orientation s in(to) the box $\hat{a}_{\vec{p}s}$ = the operator that annihilates (removes) a particle of momentum \vec{p} and spin orientation s in(from) the box

The probability amplitude for finding the particle added by $\hat{a}^+_{\vec{p}s}$ to the box at position $\vec{r}\,'$ is

$$\frac{e^{i\vec{k}\cdot\vec{r}\,'}}{\sqrt{V}} = \langle \vec{r}\,' \mid \vec{p} \rangle \tag{19.46}$$

The operator

$$\psi_{s}^{+}(\vec{r}) = \sum_{\vec{p}} \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \hat{a}_{\vec{p}s}^{+}$$
(19.47)

adds a particle to the system in a superposition of momentum states $(\hat{a}^+_{\vec{p}s})$ each with amplitude

$$\frac{e^{-ik\cdot\vec{r}}}{\sqrt{V}}\tag{19.48}$$

This implies that the probability amplitude for finding the particle added to the box by $\psi_s^+(\vec{r})$ at the position \vec{r}' is

$$\langle \vec{r}\,' | \sum_{\vec{p}} \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \hat{a}^{+}_{\vec{p}s} |0\rangle = \sum_{\vec{p}} \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \langle \vec{r}\,' | \vec{p}\rangle$$

$$= \sum_{\vec{p}} \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \frac{e^{-i\vec{k}\cdot\vec{r}\,'}}{\sqrt{V}} = \delta(\vec{r} - \vec{r}\,')$$

$$(19.49)$$

This says that the operator $\psi^+_s(\vec{r})$ adds all the amplitude at the position \vec{r} or we say

 $\psi^+_s(\vec{r}) \; \mathrm{adds}(\mathit{creates})$ a particle at position \vec{r} with spin orientation s

In a similar manner, the operator

$$\psi_s(\vec{r}) = (\psi_s^+(\vec{r}))^+ \sum_{\vec{p}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \hat{a}_{\vec{p}s}$$
(19.50)

removes (annihilates) a particle at point \vec{r} .

The
$$\psi_s^+(\vec{r})$$
 and $\psi_s(\vec{r})$ are called *field operators*.

In this new formalism, position and momentum are *once again just numbers*, but the wave functions are *now* operators. Hence the name *second quantization*.

For bosons we have

$$[\psi_s(\vec{r}), \psi_{s'}(\vec{r}')] = 0 = [\psi_s^+(\vec{r}), \psi_{s'}^+(\vec{r}')]$$
(19.51)

and for fermions we have

$$\{\psi_s(\vec{r}), \psi_{s'}(\vec{r}')\} = 0 = \{\psi_s^+(\vec{r}), \psi_{s'}^+(\vec{r}')\}$$
(19.52)

These relations imply that

for bosons adding (removing) a particle at \vec{r} is an operation that *commutes* with adding(removing) a particle at \vec{r}'

and

for fermions adding(removing) a particle at \vec{r} is an operation that *anticommutes* with adding(removing) a particle at \vec{r}' (change of sign)

Finally, for bosons we get

$$\begin{bmatrix} \psi_{s}(\vec{r}), \psi_{s'}^{+}(\vec{r}\,') \end{bmatrix} = \sum_{\vec{p}\vec{p}'} \frac{e^{i\vec{k}\cdot\vec{r}}e^{-i\vec{k}\cdot\vec{r}\,'}}{V} \begin{bmatrix} \hat{a}_{\vec{p}s}, \hat{a}_{\vec{p}\,'s'}^{+} \end{bmatrix}$$
$$= \sum_{\vec{p}\vec{p}\,'} \frac{e^{i\vec{k}\cdot\vec{r}}e^{-i\vec{k}\cdot\vec{r}\,'}}{V} \delta_{\vec{p}\vec{p}\,'}\delta_{ss'} = \delta(\vec{r}-\vec{r}\,')\delta_{ss'}$$
(19.53)

and similarly for fermions we get

$$\{\psi_{s}(\vec{r}),\psi_{s'}^{+}(\vec{r}\,')\} = \sum_{\vec{p}\vec{p}\,'} \frac{e^{i\vec{k}\cdot\vec{r}}e^{-i\vec{k}\cdot\vec{r}\,'}}{V} \{\hat{a}_{\vec{p}s},\hat{a}_{\vec{p}\,'s'}^{+}\}$$
$$= \sum_{\vec{p}\vec{p}\,'} \frac{e^{i\vec{k}\cdot\vec{r}}e^{-i\vec{k}\cdot\vec{r}\,'}}{V} \delta_{\vec{p}\vec{p}\,'}\delta_{ss'} = \delta(\vec{r}-\vec{r}\,')\delta_{ss'}$$
(19.54)

These relations imply that creating particles commutes(bosons) or anticommutes(fermions) with annihilating particles unless the two, operations occur at the *same point* in space. In this case, if there are no particles at \vec{r} , then

$$\psi_s^+(\vec{r})\psi_s(\vec{r}) \to 0 \tag{19.55}$$

i.e., we cannot annihilate a particle at a point if none exists there.

On the other hand

$$\psi_s(\vec{r})\psi_s^+(\vec{r}) \text{ does not } \to 0$$
 (19.56)

since $\psi_s^+(\vec{r})$ adds a particle that $\psi_s(\vec{r})$ then removes!

Suppressing spin indices for simplicity, the state vector

$$|\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n\rangle = \frac{1}{\sqrt{n!}} \psi^+(\vec{r}_n) \dots \psi^+(\vec{r}_2) \psi^+(\vec{r}_1) |0\rangle$$
(19.57)

represents the state with one particle at \vec{r}_1 , one particle at \vec{r}_2 , and so on.

We will use these states as a basis for the many particle, many level system. The states have the properties:

1. for bosons

$$|\vec{r}_2, \vec{r}_1, \dots, \vec{r}_n\rangle = |\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n\rangle$$
 (19.58)

due to the commutation relations which imply

$$\psi^{+}(\vec{r}_{1})\psi^{+}(\vec{r}_{2}) = \psi^{+}(\vec{r}_{2})\psi^{+}(\vec{r}_{1})$$
(19.59)

2. for fermions

$$|\vec{r}_2, \vec{r}_1, \dots, \vec{r}_n\rangle = -|\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n\rangle$$
 (19.60)

due to the anticommutation relations which imply

$$\psi^{+}(\vec{r}_{1})\psi^{+}(\vec{r}_{2}) = -\psi^{+}(\vec{r}_{2})\psi^{+}(\vec{r}_{1})$$
(19.61)

Since

$$\psi^{+}(\vec{r}) | \vec{r}_{1}, \vec{r}_{2}, \dots, \vec{r}_{n} \rangle = \frac{\sqrt{n+1}}{\sqrt{n+1!}} \psi^{+}(\vec{r}) \psi^{+}(\vec{r}_{n}) \dots \psi^{+}(\vec{r}_{2}) \psi^{+}(\vec{r}_{1}) | 0 \rangle$$
$$= \sqrt{n+1} | \vec{r}_{1}, \vec{r}_{2}, \dots, \vec{r}_{n}, \vec{r} \rangle$$
(19.62)

the commutation/anticommutation properties of the ψ^+ imply that the new state is automatically correctly symmetric or antisymmetric. This is one of the great advantages of the annihilation/creation operator formalism. We can show this important property this way:

$$\psi(\vec{r}) |\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n\rangle = \frac{1}{\sqrt{n!}} \psi(\vec{r}) \psi^+(\vec{r}_n) \dots \psi^+(\vec{r}_2) \psi^+(\vec{r}_1) |0\rangle$$
(19.63)
$$= \frac{1}{\sqrt{n!}} \left[\delta(\vec{r} - \vec{r}_n) \pm \psi^+(\vec{r}_n) \psi(\vec{r}) \right] \psi^+(\vec{r}_{n-1}) \dots \psi^+(\vec{r}_2) \psi^+(\vec{r}_1) |0\rangle$$

where

$$\pm \rightarrow \left[\begin{array}{c} bosons\\ fermions\end{array}\right] \tag{19.64}$$

We now continue commuting $\psi(\vec{r})$ with the ψ^+ 's to the right until we have

.....
$$\psi(\vec{r})|0\rangle = 0$$
 (19.65)

since $\psi(\vec{r})|0\rangle = 0$. If we actually carry out this process we obtain

$$\psi(\vec{r}) | \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n \rangle = \frac{1}{\sqrt{n!}} [\delta(\vec{r} - \vec{r}_n) | \vec{r}_1, \vec{r}_2, \dots, \vec{r}_{n-1} \rangle \\ \pm \delta(\vec{r} - \vec{r}_{n-1}) | \vec{r}_1, \vec{r}_2, \dots, \vec{r}_{n-2}, \vec{r}_n \rangle \\ + \dots + (\pm 1)^{n-1} | \vec{r}_2, \dots, \vec{r}_n \rangle]$$
(19.66)

This says that

removing a particle at \vec{r} is only possible if $\vec{r}=\vec{r}_n$ or $\vec{r}=\vec{r}_{n-1}$ or or $\vec{r}=\vec{r}_1$

and if one of these conditions is true, then

what remains is the correctly symmetrized combination of (n-1) particle states

Because $\psi^+ = (\psi)^+$, i.e., they are Hermitian conjugate operators, we have

 $\begin{array}{l} \psi(\vec{r}) \left| \vec{r}_{1}, \vec{r}_{2}, \dots, \vec{r}_{n} \right\rangle \text{ removes a particle } \\ \psi^{+}(\vec{r}) \left| \vec{r}_{1}, \vec{r}_{2}, \dots, \vec{r}_{n} \right\rangle \quad \text{adds a particle } \end{array} \right\} \text{ when acting to the right }$

but

$$\left\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n | \psi(\vec{r}) \text{ adds a particle} \\ \left\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n | \psi^+(\vec{r}) \text{ removes a particle} \right\}$$
when acting to the left (19.67)

i.e.,

$$\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n | = \left[\frac{1}{\sqrt{n!}} \psi^+(\vec{r}_n) \dots \psi^+(\vec{r}_2) \psi^+(\vec{r}_1) | 0 \rangle \right]^+$$

= $\frac{1}{\sqrt{n!}} \langle 0 | \psi(\vec{r}_1) \psi(\vec{r}_2) \dots \psi(\vec{r}_n)$ (19.68)

.

Note the *reversal in the order* of the operators.

According to these rules the basis states are normalized as follows:

$$\langle \vec{r}_1', \vec{r}_2', \dots, \vec{r}_{n'} | \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n \rangle = \frac{\delta_{nn'}}{n!} \sum_P (\pm 1)^P P \left[\delta(\vec{r}_1 - \vec{r}_1') \delta(\vec{r}_2 - \vec{r}_2') \dots \delta(\vec{r}_n - \vec{r}_n') \right]$$
(19.69)

where

$$\sum_{P} = \text{sum over all permutations if the coordinates}$$
(19.70)

and

$$(\pm)^{P} = \begin{cases} \pm 1 & \text{bosons} \\ \pm 1 & \text{fermions - even permutation} \\ \pm 1 & \text{fermions - odd permutation} \end{cases}$$
(19.71)

What is the state $|\varphi\rangle$ where the particles have a wave function $\phi(\vec{r}_1, \dots, \vec{r}_n)$?

Since the correctly symmetrized wave function must be

$$\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n \mid \varphi \rangle \tag{19.72}$$

we must have

$$|\varphi\rangle = \int d^{3}\vec{r}_{1}' d^{3}\vec{r}_{2}' \dots d^{3}\vec{r}_{n}' \phi(\vec{r}_{1}', \dots, \vec{r}_{n}') |\vec{r}_{1}', \vec{r}_{2}', \dots, \vec{r}_{n}'\rangle$$
(19.73)

which implies that

$$\langle \vec{r}_1, \vec{r}_2, ..., \vec{r}_n \mid \varphi \rangle = \frac{1}{n!} \sum_P (\pm 1)^P P \phi(\vec{r}_1, ..., \vec{r}_n)$$
 (19.74)

and thus the true wave function is properly symmetrized.

This result is true even if $\phi(\vec{r}_1, \dots, \vec{r}_n)$ is not already properly symmetrized. When it already properly symmetrized, then all n! terms are identical and

$$\langle \vec{r}_1, \vec{r}_2, ..., \vec{r}_n \mid \varphi \rangle = \phi(\vec{r}_1, ..., \vec{r}_n)$$
 (19.75)

We must have

$$\langle \varphi \mid \varphi \rangle = 1 \tag{19.76}$$

if $\phi(\vec{r}_1, \dots, \vec{r}_n)$ is symmetrized and

$$1 = \int d^3 \vec{r}_1 d^3 \vec{r}_2 \dots d^3 \vec{r}_n \phi * (\vec{r}_1, \dots, \vec{r}_n) \phi(\vec{r}_1, \dots, \vec{r}_n)$$
(19.77)

i.e.,

$$\begin{aligned} \langle \varphi \, | \, \varphi \rangle &= \int d^3 \vec{r}_1 d^3 \vec{r}_2 \dots d^3 \vec{r}_n \phi * (\vec{r}_1, \dots, \vec{r}_n) \\ &\times \langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n | \int d^3 \vec{r}_1 \, ' d^3 \vec{r}_2 \, ' \dots d^3 \vec{r}_n \, ' \phi(\vec{r}_1 \, ', \dots, \vec{r}_n \, ') \, | \vec{r}_1 \, ', \vec{r}_2', \dots, \vec{r}_n \, ' \rangle \\ &= \int d^3 \vec{r}_1 d^3 \vec{r}_2 \dots d^3 \vec{r}_n \phi * (\vec{r}_1, \dots, \vec{r}_n) \phi(\vec{r}_1 \, ', \dots, \vec{r}_n \, ') \\ &\times \frac{1}{n!} \sum_P (\pm 1)^P P \left[\delta(\vec{r}_1 - \vec{r}_1 \, ') \delta(\vec{r}_2 - \vec{r}_2 \, ') \dots \delta(\vec{r}_n - \vec{r}_n \, ') \right] \\ &= \int d^3 \vec{r}_1 d^3 \vec{r}_2 \dots d^3 \vec{r}_n \phi * (\vec{r}_1, \dots, \vec{r}_n) \phi(\vec{r}_1, \dots, \vec{r}_n) = 1 \end{aligned}$$

Now $\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n | \varphi \rangle$ is the amplitude for observing particles at $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n$. It implies that

$$|\varphi\rangle = \int d^{3}\vec{r}_{1}d^{3}\vec{r}_{2}...d^{3}\vec{r}_{n} |\vec{r}_{1},\vec{r}_{2},....,\vec{r}_{n}\rangle\langle\vec{r}_{1},\vec{r}_{2},....,\vec{r}_{n} |\varphi\rangle$$
(19.78)

which says that

$$\int d^3 \vec{r}_1 d^3 \vec{r}_2 \dots d^3 \vec{r}_n \left| \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n \right\rangle \left\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_n \right| = \hat{I}_n \tag{19.79}$$

as it should for a complete set within the *n*-particle subspace, i.e., it is \hat{I}_n only when operating on properly symmetrized *n*-particle states.

We then have for $|\varphi\rangle$ and *n*-particle states

$$\hat{I}_{n'} \left| \varphi \right\rangle = \delta_{nn'} \left| \varphi \right\rangle \tag{19.80}$$

which implies that

$$\hat{I} = \sum_{n=0}^{\infty} \hat{I}_n = |0\rangle \langle 0| + \sum_{n=1}^{\infty} \hat{I}_n$$
(19.81)

is the identity operator when acting on properly symmetrized states for any number of particles.

19.3 Second Quantized Operators

How do we write operators in this formalism?

As a first example, let us consider the operator

$$\rho(\vec{r}) = \psi^{+}(\vec{r})\psi(\vec{r})$$
(19.82)

To see what this represents physically we calculate the matrix element

$$\langle \varphi' | \rho(\vec{r}) | \varphi \rangle \tag{19.83}$$

where $|\varphi\rangle$ and $|\varphi'\rangle$ are *n*-particle states. We obtain

$$\langle \varphi' | \rho(\vec{r}) | \varphi \rangle = \langle \varphi' | \psi^{+}(\vec{r}) \psi(\vec{r}) | \varphi \rangle = \langle \varphi' | \psi^{+}(\vec{r}) \hat{I} \psi(\vec{r}) | \varphi \rangle$$

$$= \langle \varphi' | \psi^{+}(\vec{r}) \left(| 0 \rangle \langle 0 | + \sum_{n'=1}^{\infty} \hat{I}_{n'} \right) \psi(\vec{r}) | \varphi \rangle$$
(19.84)

Now the state

$$\psi(\vec{r}) |\varphi\rangle \rightarrow an (n-1) - particle state$$
 (19.85)

and therefore,

$$|0\rangle \langle 0|\psi(\vec{r})|\varphi\rangle = 0 \tag{19.86}$$

and

$$\sum_{n'=1}^{\infty} \hat{I}_{n'}\psi(\vec{r}) |\varphi\rangle = 0 \quad unless \quad n' = n-1$$
(19.87)

We thus obtain

Now, since the $\langle \vec{r}_1,...,\vec{r}_n \mid \varphi \rangle$ are completely symmetrized (or antisymmetrized) this can be written as

$$\langle \varphi' | \rho(\vec{r}) | \varphi \rangle = \int d^3 \vec{r}_1 \dots d^3 \vec{r}_n \langle \varphi' | \vec{r}_1, \dots, \vec{r}_n \rangle \sum_{i=1}^n \delta(\vec{r} - \vec{r}_i) \langle \vec{r}_1, \dots, \vec{r}_n | \varphi \rangle$$

$$= \langle \varphi' | \sum_{i=1}^n \delta(\vec{r} - \vec{r}_i) | \varphi \rangle$$

$$(19.89)$$

Since these two objects have all their matrix elements are identical, they must be equal. Therefore,

$$\rho(\vec{r}) = \sum_{i=1}^{n} \delta(\vec{r} - \vec{r}_i)$$
(19.90)

or

 $\rho(\vec{r}) = a representation of the density operator in this formalism$ The way to think about this operator is as follows:

 $\psi^+(\vec{r})\psi(\vec{r})$ tests the density of particles at \vec{r} by attempting to remove a particle located at \vec{r} and then to putting it back

If the particles have spin, the density operator for particles at \vec{r} with spin s is

$$\psi_s^+(\vec{r})\psi_s(\vec{r})$$
 (19.91)

and

$$\rho(\vec{r}) = \sum_{s} \psi_{s}^{+}(\vec{r})\psi_{s}(\vec{r}) = the total density operator$$
(19.92)

$$\hat{N} = \int d^3 \vec{r} \rho(\vec{r}) = \sum_s \int d^3 \vec{r} \psi_s^+(\vec{r}) \psi_s(\vec{r}) = total \, number \, operator \qquad (19.93)$$

This agrees with our earlier result as can be seen below:

$$\hat{N} = \sum_{s} \int d^{3}\vec{r}\psi_{s}^{+}(\vec{r})\psi_{s}(\vec{r}) = \sum_{s} \int d^{3}\vec{r} \left(\sum_{\vec{p}} \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\hat{a}_{\vec{p}s}^{+}\right) \left(\sum_{\vec{p}} \frac{e^{i\vec{k}'\cdot\vec{r}}}{\sqrt{V}}\hat{a}_{\vec{p}'s}\right)$$
$$= \sum_{s} \sum_{\vec{p}\vec{p}'} \hat{a}_{\vec{p}s}^{+} \hat{a}_{\vec{p}'s} \int d^{3}\vec{r} \frac{e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}}{V} = \sum_{s} \sum_{\vec{p}\vec{p}'} \hat{a}_{\vec{p}s}^{+} \hat{a}_{\vec{p}'s} \delta_{\vec{p}\vec{p}'} = \sum_{\vec{p}s} \hat{a}_{\vec{p}s}^{+} \hat{a}_{\vec{p}s}$$

Now to figure out other operators

Any operator that is given by the relation $f(\vec{p}_{op})$ is easily written down in this formalism, i.e., such an operator is given by the number of times \vec{p} occurs $(\hat{N}_{\vec{p}} = \hat{a}_{\vec{p}s}^+ \hat{a}_{\vec{p}s})$ times the value of the operator $(f(\vec{p}))$ summed over $(\vec{p}s)$ or

$$f(\vec{p}_{op}) = \sum_{\vec{p}s} f(\vec{p}) \hat{a}^{+}_{\vec{p}s} \hat{a}_{\vec{p}s}$$
(19.94)

Therefore, the kinetic energy operator \hat{T} is given by

$$\hat{T} = \sum_{\vec{p}s} \frac{\vec{p}^2}{2m} \hat{a}^+_{\vec{p}s} \hat{a}_{\vec{p}s}$$
(19.95)

We can rewrite this expression in a form involving the field operators that will then lead to a prescription for writing any operator in this formalism.

If we invert the equations for $\psi_s^+(\vec{r})$ and $\psi_s(\vec{r})$ we get

$$\hat{a}_{\vec{p}s}^{+} = \int d^{3}\vec{r} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \psi_{s}^{+}(\vec{r}) \quad , \quad \hat{a}_{\vec{p}s} = \int d^{3}\vec{r} \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \psi_{s}(\vec{r})$$
(19.96)

Physically, the first of this pair of equations implies that

to create a particle with momentum \vec{p} we create particles at different points \vec{r} with relative amplitudes $e^{i\vec{k}\cdot\vec{r}}/\sqrt{V}$

and so on for the second equation of the pair, which is exactly what we have been assuming all along!

Using these equations we get

$$\hat{T} = \frac{1}{2m} \frac{1}{V} \sum_{\vec{p}s} \int d^{3}\vec{r} d^{3}\vec{r}, \left(\vec{p}e^{i\vec{k}\cdot\vec{r}}\right) \cdot \left(\vec{p}e^{-i\vec{k}\cdot\vec{r},'}\right) \psi_{s}^{+}(\vec{r}) \psi_{s}(\vec{r},')$$
$$= \frac{\hbar^{2}}{2m} \frac{1}{V} \sum_{\vec{p}s} \int d^{3}\vec{r} d^{3}\vec{r}' \left(\nabla_{\vec{r}}e^{i\vec{k}\cdot\vec{r}}\right) \cdot \left(\nabla_{\vec{r},'}e^{-i\vec{k}\cdot\vec{r},'}\right) \psi_{s}^{+}(\vec{r}) \psi_{s}(\vec{r},')$$

We now integrate by parts, assuming that $\psi_s^+(\vec{r}) \to 0$ and $\psi_s(\vec{r}) \to 0$ as $r \to \infty$ so that *surface* terms $\to 0$. We get

$$\hat{T} = \frac{\hbar^2}{2m} \frac{1}{V} \sum_{\vec{p}s} \int d^3 \vec{r} d^3 \vec{r}, ' e^{i\vec{k}\cdot\vec{r}} e^{-i\vec{k}\cdot\vec{r}, '} (\nabla_{\vec{r}}\psi^+_s(\vec{r})) \cdot (\nabla_{\vec{r}, '}\psi_s(\vec{r}, '))$$
(19.97)

Using

$$\frac{1}{V} \sum_{\vec{p}s} e^{i\vec{k}\cdot\vec{r}} e^{-i\vec{k}\cdot\vec{r}\,'} = \delta(\vec{r} - \vec{r}\,') \tag{19.98}$$

and doing the $\vec{r}\,'$ integration we get

$$\hat{T} = \frac{\hbar^2}{2m} \int d^3 \vec{r} \nabla \psi^+(\vec{r}) \cdot \nabla \psi(\vec{r})$$
(19.99)

This is very *similar* to the expectation value of the kinetic energy operator for a single particle, i.e.,

$$\left\langle \hat{T} \right\rangle = \frac{\hbar^2}{2m} \int d^3 \vec{r} \nabla \phi * (\vec{r}) \cdot \nabla \phi(\vec{r})$$
(19.100)

Similarly, the density operator resembles the probability density $\phi * (\vec{r})\phi(\vec{r})$ for finding a single particle with wave function ϕ at the point \vec{r} .

This leads to the general concept of *second quantization* where

one-particle wavefunctions appear to have become operators that create/annihilate particles

single-particle expectation values appear to have become operators for physical observables

position and momentum appear to have become ordinary numbers

We can now exploit this similarity to write down other operators, for example,

the current density operator is given by

$$j(\vec{r}) = \frac{1}{2im} \left[\psi^{+}(\vec{r})(\nabla \psi(\vec{r})) - (\nabla \psi^{+}(\vec{r}))\psi(\vec{r}) \right]$$
(19.101)

the operator for the density of spin at point \vec{r} is given by

$$\vec{S}(\vec{r}) = \frac{1}{2} \sum_{ss'} \psi_s^+(\vec{r}) \vec{\sigma}_{ss'} \psi_{s'}(\vec{r})$$
(19.102)

where

$$\vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \tag{19.103}$$

19.3.1 Example - Gas of N Non-Interacting Spin 1/2 Fermions

We assume that the system is in its ground state.

As we discussed earlier, the ground state $|\varphi_0\rangle$ corresponds to all momentum states (energy levels) being filled starting from the lowest level. Since we have a finite number of particles, there will be a maximum momentum value, $p_F =$ the *Fermi momentum*.

In the new formalism, we describe the ground state via a set of occupation numbers

$$n_{\vec{p}\uparrow} = n_{\vec{p}\downarrow} = \langle \varphi_0 | \, \hat{a}^+_{\vec{p}\uparrow} \hat{a}_{\vec{p}\uparrow} | \varphi_0 \rangle = \begin{cases} 1 & |\vec{p}| \le p_F \\ 0 & |\vec{p}| \ge p_F \end{cases}$$
(19.104)

Now

$$N = \sum_{\vec{p}s} n_{\vec{p}s} = 2 \sum_{|\vec{p}| \le p_F} 1$$
(19.105)

Converting the sum to an integral we have

$$N = 2V \int_{0}^{p_{F}} \frac{d^{3}\vec{p}}{(2\pi\hbar)^{3}} = \frac{p_{F}^{3}}{3\pi^{2}\hbar^{3}}V$$
(19.106)

where we have used the properties

spacing between
$$p_x$$
 values is $\frac{2\pi\hbar}{L_x}$
spacing between p_y values is $\frac{2\pi\hbar}{L_y}$
spacing between p_z values is $\frac{2\pi\hbar}{L_z}$

which imply

$$\sum_{p_x} \rightarrow \frac{L_x}{2\pi\hbar} \int dp_x \tag{19.107}$$

and, thus,

$$\sum_{\vec{p}} \rightarrow \frac{V}{(2\pi\hbar)^3} \int d^3\vec{p} \tag{19.108}$$

We then get

$$p_F = \hbar \left(3\pi^2 n\right)^{1/3} \tag{19.109}$$

where

$$n = \frac{N}{V} = average \ particle \ density \tag{19.110}$$

The expectation value of the density operator is

$$\langle \rho(\vec{r}) \rangle = \sum_{s} \langle \varphi_{0} | \psi_{s}^{+}(\vec{r}) \psi_{s}(\vec{r}) | \varphi_{0} \rangle$$

$$= \sum_{s\vec{p}\vec{p}'} \frac{e^{-i\vec{k}\cdot\vec{r}}e^{i\vec{k}'\cdot\vec{r}}}{V} \langle \varphi_{0} | \hat{a}_{\vec{p}s}^{+}(\vec{r}) \hat{a}_{\vec{p}'s}(\vec{r}) | \varphi_{0} \rangle$$

$$(19.111)$$

Now

$$\langle \varphi_0 | \hat{a}^+_{\vec{p}s}(\vec{r}) \hat{a}_{\vec{p}'s}(\vec{r}) | \varphi_0 \rangle = \delta_{\vec{p}\vec{p}'} n_{\vec{p}s}$$
(19.112)

since if we remove a particle of momentum \vec{p} from the ground state, we can only get the ground state back if we add a particle of the same momentum \vec{p} . Where we have used

$$\hat{n}_{\vec{p}s} = \hat{a}^+_{\vec{p}s}(\vec{r})\hat{a}_{\vec{p}s}(\vec{r}) \tag{19.113}$$

Therefore,

$$\langle \rho(\vec{r}) \rangle = \frac{1}{V} \sum_{\vec{p}s} n_{\vec{p}s} = n = constant$$
(19.114)

Thus, the *density* of the non-interacting fermion gas is uniform.

A useful physical quantity is defined by

$$G_s(\vec{r} - \vec{r}') = \langle \varphi_0 | \psi_s^+(\vec{r}) \psi_s(\vec{r}') | \varphi_0 \rangle$$
(19.115)

which is

the amplitude for removing(annihilating) a particle with spin s at \vec{r}' from the ground state and then returning to the ground state by replacing(creating) a particle with spin s at \vec{r}

We have

$$G_{s}(\vec{r} - \vec{r}') = \sum_{\vec{p}\vec{p}'} \frac{e^{-i\vec{k}\cdot\vec{r}}e^{i\vec{k}'\cdot\vec{r}}}{V} \langle \varphi_{0} | \hat{a}_{\vec{p}s}^{+}(\vec{r}) \hat{a}_{\vec{p}'s}(\vec{r}) | \varphi_{0} \rangle$$

$$= \frac{1}{V} \sum_{\vec{p}\vec{p}'} \frac{e^{-i\vec{k}\cdot\vec{r}}e^{i\vec{k}'\cdot\vec{r}}}{V} \delta_{\vec{p}\vec{p}'} n_{\vec{p}s} = \frac{1}{V} \sum_{\vec{p}} e^{-i\vec{k}\cdot(\vec{r}-\vec{r}\,')} n_{\vec{p}s}$$
(19.116)

Changing to an integral we obtain

$$G_{s}(\vec{r} - \vec{r}') = \int_{0}^{p_{F}} \int \int \frac{d^{3}\vec{p}}{(2\pi\hbar)^{3}} e^{-i\vec{k}\cdot(\vec{r}-\vec{r}\,')} = \frac{1}{4\pi^{2}\hbar^{3}} \int_{0}^{p_{F}} p^{2}dp \int_{-1}^{1} d\mu e^{-ik\left|\vec{r}-\vec{r}\,'\right|\mu}$$
$$= \frac{1}{4\pi^{2}\hbar^{3}} \int_{0}^{p_{F}} p^{2}dp \left(e^{-ik\left|\vec{r}-\vec{r}\,'\right|\mu} - e^{ik\left|\vec{r}-\vec{r}\,'\right|\mu} \right)$$
$$= \frac{3n}{2} \frac{\sin x - x \cos x}{x^{3}}$$
(19.117)

where

$$x = \frac{p_F}{\hbar} \left| \vec{r} - \vec{r}' \right| \quad , \quad n = \frac{1}{3\pi^2} \frac{p_F^3}{\hbar^3} \tag{19.118}$$

As a function of x this looks as shown in Figure 19.1 below (for n = 1000) The single-particle correlation function oscillates with a characteristic period



Figure 19.1: G(x) - Single Particle Correlation Function

 $1/k_F$ under an envelope which falls to zero. We have for $\vec{r} = \vec{r}'$, $G_s(0) = n/2 =$ density of particles with spin orientation s. For small $|\vec{r} - \vec{r}'|$ we have

$$G_{s}(\vec{r} - \vec{r}') = \frac{3n}{2} \frac{\sin x - x \cos x}{x^{3}}$$

$$\approx \frac{3n}{2} \left[\frac{\left(x - \frac{x^{3}}{6} + \frac{x^{5}}{120}\right) - x\left(1 - \frac{x^{2}}{2} + \frac{x^{4}}{24}\right)}{x^{3}} \right]$$

$$\approx \frac{3n}{2} \left[\frac{\frac{1}{3}x^{3} - \frac{1}{30}x^{5}}{x^{3}} \right] = \frac{n}{2} \left(1 - \frac{x^{2}}{10}\right)$$

$$= \left[1 - \frac{1}{10} \left(\frac{p_{F} |\vec{r} - \vec{r}'|}{\hbar}\right)^{2} \right]$$
(19.119)

 $G_s(\vec{r} - \vec{r}')$ is called the one-particle density matrix.

19.4 Pair Correlation Function

As we have seen earlier, in a system of fermions, there is a tendency, due to the PEP, for particles with the same spin to avoid each other. This says that the amplitude for being close together must be small.

How do we calculate the relative probability of finding a particle at \vec{r}' if we know there is a particle at \vec{r} ?

One way is as follows:

1. Remove (mathematically) a particle with spin s at \vec{r} from the system. We

are then left in the N-1 particle state

$$|\varphi'(\vec{r},s)\rangle = \psi_s(\vec{r}) |\varphi_0\rangle \tag{19.120}$$

2. Calculate the density distribution of the particles with spin s' in the new state. The density is

$$\langle \varphi'(\vec{r},s) | \psi_{s'}^{+}(\vec{r}') \psi_{s'}(\vec{r}') | \varphi'(\vec{r},s) \rangle$$

= $\langle \varphi_{0} | \psi_{s}^{+}(\vec{r}) \psi_{s'}^{+}(\vec{r}') \psi_{s'}(\vec{r}') \psi_{s}(\vec{r}) | \varphi_{0} \rangle = \left(\frac{n}{2}\right)^{2} g_{ss'}(\vec{r} - \vec{r}')$ (19.121)

where $g_{ss'}(\vec{r} - \vec{r}') \equiv$ the pair correlation function.

An equivalent way of asking the same question is the following:

- 1. Remove(annihilate) a particle from \vec{r} using $\psi_s(\vec{r})$
- 2. Remove (annihilate) a particle from \vec{r}' using $\psi'_s(\vec{r})'$ The relative amplitude for ending up in some N-2 particle state $|\varphi''_i\rangle$ is

$$\langle \varphi_i'' | \psi_{s'}(\vec{r}\,') \psi_s(\vec{r}\,) | \varphi_0 \rangle \tag{19.122}$$

3. Sum over a complete set of N-2 particle states

This gives the total probability of removing two particles and ending up in any N-2 particle state. We get

$$\sum_{i} \left| \left\langle \varphi_{i}^{\prime\prime} \right| \psi_{s\prime}(\vec{r}\,') \psi_{s}(\vec{r}\,) \left| \varphi_{0} \right\rangle \right|^{2}$$

$$= \left\langle \varphi_{0} \right| \psi_{s}^{+}(\vec{r}\,) \psi_{s\prime}^{+}(\vec{r}\,') \sum_{i} \left| \varphi_{i}^{\prime\prime} \right\rangle \left\langle \varphi_{i}^{\prime\prime} \right| \psi_{s\prime}(\vec{r}\,') \psi_{s}(\vec{r}\,) \left| \varphi_{0} \right\rangle$$

$$= \left\langle \varphi_{0} \right| \psi_{s}^{+}(\vec{r}\,) \psi_{s\prime}^{+}(\vec{r}\,') \psi_{s\prime}(\vec{r}\,') \psi_{s}(\vec{r}\,) \left| \varphi_{0} \right\rangle = \left(\frac{n}{2} \right)^{2} g_{ss\prime}(\vec{r} - \vec{r}\,')$$

$$= \text{ total probability of removing two particles}$$
(19.123)

We can evaluate $g_{ss'}(\vec{r} - \vec{r}')$ by shifting to the creation/annihilation operator formalism. We get

$$\left(\frac{n}{2}\right)^{2} g_{ss'}(\vec{r} - \vec{r}\,') = \sum_{\vec{p}\vec{p}\,'\vec{q}\vec{q}\,'} \frac{e^{-i(\vec{p} - \vec{p}\,')\cdot\vec{r}/h} e^{-i(\vec{q} - \vec{q}\,')\cdot\vec{r}'/h}}{V^{2}} \left\langle\varphi_{0}|\hat{a}^{+}_{\vec{p}s}\hat{a}^{+}_{\vec{q}s'}\hat{a}_{\vec{q}\,'s'}\hat{a}_{\vec{p}\,'s}|\varphi_{0}\right\rangle$$
(19.124)

Now

$$\langle \varphi_0 | \hat{a}^+_{\vec{p}s}(\vec{r}\,) \hat{a}^+_{\vec{q}s'}(\vec{r}\,') \hat{a}_{\vec{q}\,'s'}(\vec{r}\,') \hat{a}_{\vec{p}\,'s}(\vec{r}\,) | \varphi_0 \rangle = 0 \tag{19.125}$$

unless we put back particles with the same spin and same momentum that we remove, i.e.,

if
$$s \neq s'$$
, then $\vec{p}' = \vec{p}$ and $\vec{q}' = \vec{q}$ (19.126)

This implies that

$$\langle \varphi_0 | \hat{a}^+_{\vec{p}s} \hat{a}^+_{\vec{q}s'} \hat{a}_{\vec{q}\,'s'} \hat{a}_{\vec{p}\,'s} | \varphi_0 \rangle = \langle \varphi_0 | \hat{a}^+_{\vec{p}s} \hat{a}_{\vec{p}s} \hat{a}^+_{\vec{q}s'} \hat{a}_{\vec{q}s'} | \varphi_0 \rangle = n_{\vec{p}s} n_{\vec{q}s'}$$
(19.127)

We then get

$$\left(\frac{n}{2}\right)^2 g_{ss'}(\vec{r} - \vec{r}') = \frac{1}{V^2} \sum_{\vec{p}\vec{q}} n_{\vec{p}s} n_{\vec{q}s'} = n_s n_{s'} = \left(\frac{n}{2}\right)^2$$
(19.128)

or

$$g_{ss'}(\vec{r} - \vec{r}') = 1 \text{ for } s \neq s'$$
 (19.129)

This implies that the relative probability for finding particles at \vec{r} and \vec{r}' for different spins is independent of $|\vec{r} - \vec{r}'|$. This is the *same result* as one obtains in a classical non-interacting gas.

The PEP does not influence particles of different(opposite in this case) spins.

On the other hand, if the spins are the same, s = s', then we have two possibilities, namely,

$$\vec{p}' = \vec{p}$$
 and $\vec{q}' = \vec{q}$ or $\vec{p}' = \vec{q}$ and $\vec{q}' = \vec{p}$

Note that if $\vec{p}\,' = \vec{q}\,'$, then $\langle \varphi_0 | \, \hat{a}^+_{\vec{p}s} \hat{a}^+_{\vec{q}s} \hat{a}_{\vec{q}\,'s} \hat{a}_{\vec{p}\,'s} | \varphi_0 \rangle = 0$ since

$$\hat{a}_{\vec{q}'s}\hat{a}_{\vec{p}'s} \to (\hat{a}_{\vec{p}'s})^2 = 0 \qquad \text{(for fermions)} \qquad (19.130)$$

Therefore, we have

We must use the superposition of both (indistinguishable)possibilities.

This becomes

$$\langle \varphi_0 | \hat{a}^+_{\vec{p}s} \hat{a}^+_{\vec{q}s} \hat{a}_{\vec{q}'s} \hat{a}_{\vec{p}'s} | \varphi_0 \rangle = (\delta_{\vec{p}\vec{p}'} \delta_{\vec{q}\vec{q}'} - \delta_{\vec{p}\vec{q}'} \delta_{\vec{q}\vec{p}'}) \langle \varphi_0 | \hat{a}^+_{\vec{p}s} \hat{a}_{\vec{p}s} \hat{a}^+_{\vec{q}s} \hat{a}_{\vec{q}s} | \varphi_0 \rangle$$

$$= (\delta_{\vec{p}\vec{p}'} \delta_{\vec{q}\vec{q}'} - \delta_{\vec{p}\vec{q}'} \delta_{\vec{q}\vec{p}'}) n_{\vec{p}s} n_{\vec{q}s}$$
(19.132)

where we have used the anticommutation relations for fermion operators

$$\vec{q} \neq \vec{p} \qquad \left\{ \hat{a}_{\vec{p}s}, \hat{a}^+_{\vec{q}s} \right\} = 0 = \left\{ \hat{a}_{\vec{p}s}, \hat{a}_{\vec{q}s} \right\}$$
$$\vec{q} = \vec{p} \qquad \left\langle \dots \right\rangle = 0$$

We finally obtain

$$\left(\frac{n}{2}\right)^{2} g_{ss'}(\vec{r} - \vec{r}\,') = \frac{1}{V^{2}} \sum_{\vec{p} \neq \vec{q}} \left[1 - e^{-i(\vec{p} - \vec{q}\,') \cdot (\vec{r} - \vec{r}\,')/\hbar}\right] n_{\vec{p}s} n_{\vec{q}s}$$
$$= \left(\frac{n}{2}\right)^{2} - \left[G_{s}(\vec{r} - \vec{r}\,')\right]^{2}$$
(19.133)

where $G_s(\vec{r} - \vec{r}')$ is the single particle density function. This then becomes

$$g_{ss'}(\vec{r} - \vec{r}') = 1 - \frac{9}{x^6} \left(\sin x - x \cos x\right)^2$$
(19.134)

where

$$x = \frac{p_F}{\hbar} \left| \vec{r} - \vec{r}' \right| \tag{19.135}$$

As a function of x this looks as shown in Figure 19.2 below.



Figure 19.2: g(x) - Two Particle Correlation Function - Fermions

This result implies a substantial reduction in the probability for finding two fermions of the same spin at distances less than \hbar/p_F .

The PEP causes large *correlations* in the motion of the particles with the same spin. It seems like fermions of the same spin *repel* each other at short distances. This effective repulsion is *due* to the exchange symmetry (PEP) of the wave function and *not* from any real additional potentials.

At large $|\vec{r} - \vec{r}'|$, $g_{ss} \rightarrow g_{ss'} = 1$ as we might have guessed since at large separations the PEP should have no effect and spin effects should drop out.

What happens if we consider a system of non-interacting bosons instead?

Suppose the system is in the state

$$|\varphi\rangle = |n_{\vec{p}_0}, n_{\vec{p}_1}, \dots, \rangle \tag{19.136}$$

The density in this state is

$$\langle \varphi | \psi^{+}(\vec{r})\psi(\vec{r}) | \varphi \rangle = \frac{1}{V} \sum_{\vec{p}} n_{\vec{p}} = n \qquad (19.137)$$

The calculation of the pair correlation function is the same as for fermions up to this point.

$$n^{2}g(\vec{r}-\vec{r}\,') = \sum_{\vec{p}\vec{p}\,'\vec{q}\vec{q}\,'} \frac{e^{-i(\vec{p}-\vec{p}\,')\cdot\vec{r}/\hbar}e^{-i(\vec{q}-\vec{q}\,')\cdot\vec{r}'/\hbar}}{V^{2}} \left\langle \varphi_{0} | \hat{a}_{\vec{p}}^{\dagger} \hat{a}_{\vec{q}}^{\dagger} \hat{a}_{\vec{q}\,'} \hat{a}_{\vec{p}\,'} | \varphi_{0} \right\rangle$$
(19.138)

In this case,

$$\langle \varphi_0 | \, \hat{a}^+_{\vec{p}} \hat{a}^+_{\vec{q}} \hat{a}_{\vec{q}'} \hat{a}_{\vec{p}'} | \varphi_0 \rangle \neq 0 \tag{19.139}$$

only if

$$\vec{p} = \vec{p}', \ \vec{q} = \vec{q}' \quad or \quad \vec{p} = \vec{q}', \ \vec{q} = \vec{p}'$$

These two cases are *not* distinct if $\vec{p} = \vec{q}$.

Therefore, in the same manner as before, we have

$$\begin{aligned} \left\langle \varphi_{0} \right| \hat{a}_{\vec{p}}^{\dagger} \hat{a}_{\vec{q}}^{\dagger} \hat{a}_{\vec{q}} \cdot \hat{a}_{\vec{p}'} \left| \varphi_{0} \right\rangle \\ &= \left(1 - \delta_{\vec{p}\vec{q}} \right) \left[\delta_{\vec{p}\vec{p}'} \delta_{\vec{q}\vec{q}'} \left\langle \varphi_{0} \right| \hat{a}_{\vec{p}}^{\dagger} \hat{a}_{\vec{q}}^{\dagger} \hat{a}_{\vec{p}} \left| \varphi_{0} \right\rangle + \delta_{\vec{p}\vec{q}'} \delta_{\vec{q}\vec{p}'} \left\langle \varphi_{0} \right| \hat{a}_{\vec{p}}^{\dagger} \hat{a}_{\vec{q}}^{\dagger} \hat{a}_{\vec{p}} \right| \left\langle \varphi_{0} \right\rangle \\ &+ \delta_{\vec{p}\vec{q}} \delta_{\vec{p}\vec{p}'} \delta_{\vec{q}\vec{q}'} \left\langle \varphi_{0} \right| \hat{a}_{\vec{p}}^{\dagger} \hat{a}_{\vec{p}}^{\dagger} \hat{a}_{\vec{p}} \hat{a}_{\vec{p}} \left| \varphi_{0} \right\rangle \\ &= \left(1 - \delta_{\vec{p}\vec{q}} \right) \left(\delta_{\vec{p}\vec{p}'} \delta_{\vec{q}\vec{q}'} + \delta_{\vec{p}\vec{q}'} \delta_{\vec{q}\vec{p}'} \right) n_{\vec{p}} n_{\vec{q}} + \delta_{\vec{p}\vec{q}} \delta_{\vec{p}\vec{p}'} \delta_{\vec{q}\vec{q}'} n_{\vec{p}} (n_{\vec{p}} - 1) \end{aligned} \tag{19.140}$$

where we have used $\left[\hat{a}_{\vec{p}},\hat{a}^{+}_{\vec{p}}\right] = 1$ in the last term. Therefore, we obtain

$$n^{2}g(\vec{r} - \vec{r}') = \langle \varphi | \psi^{+}(\vec{r})\psi^{+}(\vec{r}')\psi(\vec{r}')\psi(\vec{r}) | \varphi \rangle$$
$$= n^{2} + \left| \frac{1}{V} \sum_{\vec{p}} n_{\vec{p}} e^{-i\vec{k} \cdot (\vec{r} - \vec{r}')} \right|^{2} - \frac{1}{V^{2}} \sum_{\vec{p}} n_{\vec{p}}(n_{\vec{p}} + 1)$$
(19.141)

This *differs* from the fermion result in

- 1. the sign of the second term (+ instead of –), which is due to different exchange symmetry properties.
- 2. the existence of the third term, which is due to the fact that we can have many bosons in the same state.

If all the particles are in only one state, \vec{p}_0 , then we have

$$n^{2}g(\vec{r} - \vec{r}') = \langle \varphi | \psi^{+}(\vec{r})\psi^{+}(\vec{r}')\psi(\vec{r}')\psi(\vec{r}) | \varphi \rangle$$

= $n^{2} + n^{2} - \frac{1}{V^{2}}N(N+1) = \frac{N(N-1)}{V^{2}}$ (19.142)

The pair distribution function is position independent. The above result implies that the relative amplitude for removing the first particle is N/V, while the amplitude for removing a second particle is (N-1)/V since there are only N-1 remaining after removing the first particle.

Now suppose that

$$n_{\vec{p}}$$
 = smoothly varying distribution = $Ce^{-\frac{\alpha(\vec{p}-\vec{p}_0)^2}{2}}$ (19.143)

This could be a beam of particles of momentum centered at \vec{p}_0 with a Gaussian spread about \vec{p}_0 .

If we let $V \rightarrow large$, with N/V = n fixed, then the third term is of order 1/V smaller than the first two terms and we can neglect it.

Converting the remaining terms to integrals we have

$$n^{2}g(\vec{r} - \vec{r}') = \langle \varphi | \psi^{+}(\vec{r})\psi^{+}(\vec{r}')\psi(\vec{r}')\psi(\vec{r}) | \varphi \rangle$$

= $n^{2} + \left| \int \frac{d^{3}\vec{p}}{(2\pi\hbar)^{3}} n_{\vec{p}} e^{-i\vec{k}\cdot(\vec{r}-\vec{r}')} \right|^{2} = n^{2} \left[1 + e^{-\frac{(r-r')^{2}}{\alpha}} \right]$ (19.144)

A plot of this result is shown in Figure 19.3 below.



Figure 19.3: g(r) - Two Particle Correlation Function - Bosons

The $e^{-(\vec{r}-\vec{r}')^2/\alpha}$ term is due to exchange symmetry. In this case, exchange symmetry *increases* the probability that two bosons *will be found* at small separations.

In fact,

the probability of finding two bosons on top of each other is equal to *two times* the probability of finding two bosons with a large separation

19.5 Hanbury-Brown and Twiss Experiment

Do bosons really tend to clump together?

At this point we will discuss the Hanbury-Brown and Twiss(HBT) experiment that shows that they do tend to clump. The HBT experiment measures the probability of observing 2 photons simultaneously at different points in a beam of incoherent light. Incoherent light, as we saw earlier, can be described in terms of occupation numbers of photon states. The apparatus is shown in Figure 19.4 below.



Figure 19.4: Hanbury-Brown and Twiss Boson Clumping Experiment

The half-silvered mirror splits the beam into two identical beams. The amplitude for a photon to be transmitted/reflected by the mirror is $1/\sqrt{2}$ (the probability is 1/2).

HBT measured the following

 $I_1(t)$ = light intensity at detector 1 at time t $I_2(t + \tau)$ = light intensity at detector 2 at a later time $t + \tau$

and then they averaged the quantity $I_1(t)I_2(t+\tau)$ over t, keeping τ fixed.

This is the *same* as measuring the relative probability of observing two photons separated by a distance $c\tau$ in the beams (c = speed of light).

The experimental result is just $g(\vec{r} - \vec{r}')$ for $|\vec{r} - \vec{r}'| = c\tau$. This confirmed the

theory or so one thought at that time.

We ask the following question: Is this experiment a verification of the quantum mechanical theory for identical bosons? The answer might, in fact, be no!

Can we understand the result completely using classical electromagnetic theory and wave superposition? The experiment might imply that the boson properties of the photon follow from the superposition principle obeyed by classical fields and we might not need the quantum mechanical concept of a photon in this experiment.

Let us see how. Consider the setup shown in Figure 19.5 below:



Figure 19.5: Classical or Quantum?

We have two sources of photons, A and B. A emits coherent light with amplitude α and wave number k. B emits coherent light with amplitude β and wave number k'. We assume that the relative phase of the two coherent beams is *random* and that they have the *same* polarization.

The amplitude for light $(A \to 1) \to \alpha e^{ikr_1}$ and the amplitude for light $(B \to 1) \to \beta e^{ik'r'_1}$. Therefore, the superposition principle implies that

$$a_{1} = \text{ total amplitude at detector 1}$$
$$= \alpha e^{ikr_{1}} + \beta e^{ik'r'_{1}}$$
(19.145)

and that

$$I_{1} = \text{ intensity at detector } 1$$
$$= \left| \alpha e^{ikr_{1}} + \beta e^{ik'r_{1}'} \right|^{2} = |\alpha|^{2} + |\beta|^{2} + 2Real\left(\alpha * \beta e^{i(k'r_{1}'-kr_{1})} \right)$$
(19.146)

Therefore,

$$I_1 = I_1 \text{ averaged over the random phase}$$
$$= |\alpha|^2 + |\beta|^2$$
(19.147)

Similarly,

$$a_{2} = \text{ total amplitude at detector } 2$$
$$= \alpha e^{ikr_{2}} + \beta e^{ik'r_{2}'}$$
(19.148)

and that

$$I_{1} = \text{ intensity at detector } 2$$
$$= \left| \alpha e^{ikr_{2}} + \beta e^{ik'r_{2}'} \right|^{2} = |\alpha|^{2} + |\beta|^{2} + 2Real\left(\alpha * \beta e^{i(k'r_{2}'-kr_{2})} \right)$$
(19.149)

Therefore,

$$\bar{I}_1 = I_2$$
 averaged over the random phase
= $|\alpha|^2 + |\beta|^2$ (19.150)

The product of the averaged intensities $\bar{I}_1 \bar{I}_2$ is clearly *independent* of the separation distance between the two detectors.

The product of the intensities, however, behaves very differently, however, i.e.,

$$I_{1}I_{2} = |a_{1}a_{2}|^{2}$$
$$= \left|\alpha^{2}e^{ik(r_{1}+r_{2})} + \beta^{2}e^{ik'(r_{1}'+r_{2}')} + \alpha\beta\left(e^{ikr_{1}}e^{ik'r_{2}'} + e^{ik'r_{1}'}e^{ikr_{2}}\right)\right|^{2}$$
(19.151)

Multiplying out and averaging over the random phases of α and β eliminates the terms proportional to $\alpha\beta |\alpha^2|$ and $\alpha\beta |\beta^2|$, etc and we get

$$\overline{I_{1}I_{2}} = |\alpha|^{4} + |\beta|^{4} + |\alpha|^{2} |\beta|^{2} \left| e^{ikr_{1}} e^{ik'r'_{2}} + e^{ik'r'_{1}} e^{ikr_{2}} \right|^{2}$$
$$= \overline{I_{1}}\overline{I_{2}} + 2|\alpha|^{2} |\beta|^{2} \cos \left[k'(r'_{1} - r'_{2}) - k(r_{1} - r_{2}) \right]$$
(19.152)

For well-collimated beams $r'_1 - r'_2 \approx r_1 - r_2$, which gives

$$\overline{I_1 I_2} = \overline{I_1} \overline{I_2} + 2 |\alpha|^2 |\beta|^2 \cos\left[(k' - k)(r_1 - r_2)\right]$$
(19.153)

Therefore, the correlated intensities have a term that *depends* on the detector separation.

This term is a maximum when the detectors are at the same point.

If we average over all the different k and k' present in the beam (using a Gaussian distribution) we get the same form as the quantum result.

This seems to imply that the *photon bunching* effect seen in the HBT experiment is a consequence of the superposition principle applied to light from noisy sources.

The quantum mechanical interpretation of the classical result is

1st term = amplitude for both photons from A 2nd term = amplitude for both photons from B 3rd term = amplitude for one photon from A and the other from B

There are two ways to do this

1. $A \rightarrow 1$, $B \rightarrow 2$

2. $A \rightarrow 2$, $B \rightarrow 1$

These two ways are indistinguishable and the interference between them gives the cosine term.

So, we corroborate superposition and bunching, but we do not seem to need the quantum concept of a photon to do it. When one studies this problem in more detail one can prove that a photon with quantum properties must exist.

19.6 The Hamiltonian

Finally, we write the Hamiltonian in second quantized form.
Suppose the particles interact via a two-particle potential $V(\vec{r} - \vec{r}')$. The interaction energy operator then becomes

$$\nu = \frac{1}{2} \sum_{ss'} \int d^3 \vec{r} d^3 \vec{r}' V(\vec{r} - \vec{r}') \psi_s^+(\vec{r}) \psi_{s'}^+(\vec{r}') \psi_{s'}(\vec{r}') \psi_s(\vec{r})$$
(19.154)

The order of the operators in this expression is very important. This form for ν can be confirmed by comparing its matrix elements to the matrix elements in the standard formalism.

We interpret ν in this way:

- 1. it tries to remove particles from \vec{r} and $\vec{r}\,'$
- 2. if successful it counts $V(\vec{r} \vec{r}')$ and then replaces the particles
- 3. it replaces the last particle removed first
- 4. it sums over all pairs (the factor 1/2 avoids double counting of pairs) of points \vec{r} and $\vec{r}\,'$

The second quantized Hamiltonian for particles of mass m with such a pairwise interaction potential is then

$$H = \sum_{s} \int d^{3}\vec{r} \frac{\hbar^{2}}{2m} \nabla \psi_{s}^{+}(\vec{r}) \cdot \nabla \psi_{s}(\vec{r}) + \frac{1}{2} \sum_{ss'} \int d^{3}\vec{r} d^{3}\vec{r}' V(\vec{r} - \vec{r}') \psi_{s}^{+}(\vec{r}) \psi_{s'}^{+}(\vec{r}') \psi_{s'}(\vec{r}') \psi_{s}(\vec{r})$$
(19.155)

We now calculate the ground state energy of our gas of spin = 1/2 fermions.

We will treat the interaction potential as a perturbation. To lowest (zeroth) order we have

$$E^{(0)} = T = \sum_{\vec{p}s} \frac{p^2}{2m} n_{\vec{p}} = 2 \sum_{\vec{p}} \frac{p^2}{2m} = 2V \int_0^{p_F} \frac{d^3 \vec{p}}{(2\pi\hbar)^3} \frac{p^2}{2m}$$
$$= \frac{3}{5} \frac{p_F^2}{2m\hbar^2} N = \frac{3}{5} E_F$$
(19.156)

The first order energy correction $E^{(1)}$ is the expectation value of ν in the unperturbed ground state. We get

$$E^{(1)} = \frac{1}{2} \int d^{3}\vec{r} d^{3}\vec{r}' V(\vec{r} - \vec{r}') \sum_{ss'} \langle \varphi_{0} | \psi_{s}^{+}(\vec{r}) \psi_{s'}(\vec{r}') \psi_{s'}(\vec{r}') \psi_{s}(\vec{r}) | \varphi_{0} \rangle$$

$$= \frac{1}{2} \int d^{3}\vec{r} d^{3}\vec{r}' V(\vec{r} - \vec{r}') \sum_{ss'} \left(\frac{n}{2}\right)^{2} g_{ss'}(\vec{r} - \vec{r}')$$

$$= \frac{1}{2} \int d^{3}\vec{r} d^{3}\vec{r}' V(\vec{r} - \vec{r}') \left[n^{2} - \sum_{s} G_{s}^{2}(\vec{r} - \vec{r}')\right]$$
(19.157)

If we let

$$v_0 = \int d^3 \vec{r} V(\vec{r})$$
 (19.158)

then we have

$$\frac{1}{2} \int d^3 \vec{r} d^3 \vec{r}' V(\vec{r} - \vec{r}') n^2 = \frac{N n v_0}{2}$$
(19.159)

This is the average interaction of a uniform density of particles with itself (no correlations). It is called the *direct or Hartree* energy.

The second term represents the *exchange* energy

$$E_{ex} = -\frac{1}{2} \int d^3 \vec{r} d^3 \vec{r}' V(\vec{r} - \vec{r}') \sum_s G_s^2(\vec{r} - \vec{r}')$$
(19.160)

This term takes account of the *tendency* of particles of the same spin to stay apart. The effects of the short-range part of $V(\vec{r} - \vec{r}')$ are overcorrected in the direct energy and fixed up in exchange energy.

We have

$$\frac{E_{ex}}{N} = -\frac{9n}{4} \int d^3r \frac{\left(\sin\frac{p_Fr}{\hbar} - \frac{p_Fr}{\hbar}\cos\frac{p_Fr}{\hbar}\right)^2}{\left(\frac{p_Fr}{\hbar}\right)^6} V(r)$$
(19.161)

and to first order

$$E_0 = \frac{3}{5} \frac{p_F^2}{2m} + \frac{nv_0}{2} + \frac{E_{ex}}{N}$$
(19.162)

19.6.1 An Example

Consider a gas of electrons of average density ? interacting via a Coulomb potential

$$V(\vec{r} - \vec{r}') = \frac{e^2}{|\vec{r} - \vec{r}'|}$$
(19.163)

The conduction electrons in a metal form such a gas.

We note that in a real physical system of this type, we never have an isolated electron gas. There always exists enough positive charges to make the overall system electrically neutral.

To first approximation in a metal or a plasma we can replace the positive ions by a uniform background of positive charge of density +ne.

The electrostatic self-energy of this background

$$\frac{1}{2} \int d^3r d^3r' \frac{e^2 n^2}{|\vec{r} - \vec{r}'|} \tag{19.164}$$

plus the average electrostatic interaction between the positive background and the electrons

$$-\int d^3r d^3r' \frac{e^2 n^2}{|\vec{r} - \vec{r}'|} \tag{19.165}$$

exactly cancels the Hartree energy as it must because the electrostatic energy of a neutral system can only be proportional to the volume for a large system(not a higher power of the volume!).

Therefore, the net interaction energy of the electron gas (to first order) is

$$\frac{E_{ex}}{N} = -\frac{9\pi ne^2}{p_F^2} \int_0^\infty \frac{dx}{x^5} \left(\sin x - x\cos x\right)^2$$
(19.166)

For a typical electron gas, this energy is written in terms of a parameter

$$r_s = \frac{d}{a_0} = \frac{\text{average interparticle spacing}}{\text{Bohr radius}}$$
 (19.167)

Now, we also have

$$a_0 = \frac{\hbar^2}{me^2}$$
 , $n\left(\frac{4\pi}{3}d^3\right) = 1$ (19.168)

Therefore,

$$r_s = \left(\frac{9\pi}{4}\right)^{1/3} \frac{me^2}{p_F} \tag{19.169}$$

and

$$E = \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right) \frac{e^2}{a_0}$$
(19.170)

where the first term is the kinetic energy and the second term is the exchange energy.

Finally, if we write ν in the creation/annihilation operator formalism we get

$$v = \frac{1}{2V} \sum_{\vec{p}\vec{p}'} \sum_{\vec{q}\vec{q}'} \sum_{ss'} \tilde{V}_{\vec{p}'-\vec{p}} \delta_{\vec{p}+\vec{q},\vec{p}'+\vec{q}'} \hat{a}^+_{\vec{p}'s} \hat{a}^+_{\vec{q}'s'} \hat{a}_{\vec{q}s'} \hat{a}_{\vec{p}s}$$
(19.171)

where

$$\tilde{V}_{\vec{k}} = \int d^3 r \, e^{-i\vec{k}\cdot\vec{r}} V(\vec{r})$$
(19.172)

This is a sum over scattering processes. Feynman developed a clever diagrammatic method of thinking about such terms.

- 1. The delta-function represents conservation of energy and momentum in the scattering process.
- 2. The process itself is represented by the diagram in Figure 19.6 below.

We shall return to this idea later in Chapter 21 and develop a method of thinking about the universe as expressed by these diagrams.



Figure 19.6: Feynman Diagram

19.7 Bogoliubov Transformation, Quasiparticles and Superfluidity

Let us consider a weakly interacting Bose gas. From our earlier discussions we have, in general,

$$v = \frac{1}{2V} \sum_{\vec{p}\vec{p}'} \sum_{\vec{q}\vec{q}'} V_{\vec{p}'-\vec{p}} \delta_{\vec{p}+\vec{q},\vec{p}'+\vec{q}'} \hat{a}^{+}_{\vec{p}'} \hat{a}^{+}_{\vec{q}'} \hat{a}_{\vec{q}} \hat{a}_{\vec{p}}$$
$$= \frac{1}{2V} \sum_{\vec{k}\vec{p}} \sum_{\vec{q}} V_{\vec{q}} \hat{a}^{+}_{\vec{k}+\vec{q}} \hat{a}^{+}_{\vec{k}-\vec{q}} \hat{a}_{\vec{p}} \hat{a}_{\vec{q}}$$
(19.173)

so that

$$\hat{H} = \sum_{\vec{k}} \hbar \omega_{\vec{k}} \hat{a}_{\vec{k}}^{\dagger} \hat{a}_{\vec{k}} + \frac{1}{2V} \sum_{\vec{k}\vec{p}} \sum_{\vec{q}} V_{\vec{q}} \hat{a}_{\vec{k}+\vec{q}}^{\dagger} \hat{a}_{\vec{p}-\vec{q}}^{\dagger} \hat{a}_{\vec{p}} \hat{a}_{\vec{k}}$$
(19.174)

where we have used the delta function (which corresponds to momentum conservation). This corresponds to the process

$$\vec{k} + \vec{p} \to (\vec{k} + \vec{q}) + (\vec{p} - \vec{q})$$
 (19.175)

or we have momentum transfer of \vec{q} between the two interacting bosons.

At low temperatures, a Bose-Einstein condensation takes place in the $\vec{k} = 0$ mode, i.e., the $\vec{k} = 0$ mode is macroscopically occupied or

$$N_0 = \langle \Phi_0 | a^+ a | \Phi_0 \rangle \approx N \quad , \quad N - N_0 = \# excited \ particles << N_0 \qquad (19.176)$$

This means that we can neglect the interaction of excited particles with one another and restrict our attention to the interaction of the excited particles with the condensed particles.

This gives

$$\begin{aligned} \hat{H} &= \sum_{\vec{k}} \hbar \omega_{\vec{k}} \hat{a}_{\vec{k}}^{\dagger} \hat{a}_{\vec{k}} + \frac{1}{2V} V_0 \hat{a}_0^{\dagger} \hat{a}_0^{\dagger} \hat{a}_0 \hat{a}_0 \\ &+ \frac{1}{V} \sum_{\vec{k} \neq 0} \left(V_0 + V_{\vec{k}} \right) \hat{a}_0^{\dagger} \hat{a}_0 \hat{a}_{\vec{k}}^{\dagger} \hat{a}_{\vec{k}} + \frac{1}{2V} \sum_{\vec{k} \neq 0} V_{\vec{k}} \left(\hat{a}_{\vec{k}}^{\dagger} \hat{a}_{-\vec{k}}^{\dagger} \hat{a}_0 \hat{a}_0 + \hat{a}_0^{\dagger} \hat{a}_0^{\dagger} \hat{a}_{\vec{k}} \hat{a}_{-\vec{k}} \right) + \dots \end{aligned}$$

$$(19.177)$$

The effect of \hat{a}_0^+ and \hat{a}_0 on the state with N_0 particles in the condensate is

$$\hat{a}_0 |...., N_0,\rangle = \sqrt{N_0} |...., N_0 - 1,\rangle$$
 (19.178)

$$\hat{a}_0^+ |...., N_0,\rangle = \sqrt{N_0 + 1} |...., N_0 + 1,\rangle$$
 (19.179)

Since N_0 is a very large number ($\approx 10^{23}$), both of these relations correspond to multiplication by $\sqrt{N_0}$. It is physically clear that the removal or addition of one particle from the condensate will make no difference to the physical properties of the system.

In comparison to N_0 , the effect of the commutator $[\hat{a}_0, \hat{a}_0^+] = 1$ is negligible. This says that, in this case, the operators \hat{a}_0^+ and \hat{a}_0 can be approximated by a number $\sqrt{N_0}$.

We then have

$$\hat{H} = \sum_{\vec{k}\neq 0} \frac{\hbar^2 k^2}{2m} \hat{a}_{\vec{k}}^+ \hat{a}_{\vec{k}} + \frac{1}{2V} N_0^2 V_0 + \frac{N_0}{V} \sum_{\vec{k}\neq 0} \left(V_0 + V_{\vec{k}} \right) \hat{a}_{\vec{k}}^+ \hat{a}_{\vec{k}} + \frac{N_0}{2V} \sum_{\vec{k}\neq 0} V_{\vec{k}} \left(\hat{a}_{\vec{k}}^+ \hat{a}_{-\vec{k}}^+ + \hat{a}_{\vec{k}} \hat{a}_{-\vec{k}} \right)$$
(19.180)

We can write

$$N = N_0 + \sum_{\vec{k} \neq 0} \hat{a}^+_{\vec{k}} \hat{a}_{\vec{k}}$$
(19.181)

which says that (carrying out the necessary algebra)

$$\frac{1}{2V}N_0^2 V_0 = \frac{1}{2V}N^2 V_0 + \frac{N}{V}\sum_{\vec{k}\neq 0}V_{\vec{k}}\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}} + \frac{V_0}{2V}\sum_{\vec{k},\vec{k}'\neq 0}\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}\hat{a}^+_{\vec{k}'}\hat{a}_{\vec{k}'}$$
(19.182)

The Hamiltonian then becomes

$$\hat{H} = \sum_{\vec{k}\neq 0} \frac{\hbar^2 k^2}{2m} \hat{a}^+_{\vec{k}} \hat{a}^-_{\vec{k}} + \frac{N}{V} \sum_{\vec{k}\neq 0} V_{\vec{k}} \hat{a}^+_{\vec{k}} \hat{a}^-_{\vec{k}} + \frac{N^2}{2V} V_0 + \frac{N}{2V} \sum_{\vec{k}\neq 0} V_{\vec{k}} (\hat{a}^+_{\vec{k}} \hat{a}^+_{-\vec{k}} + \hat{a}^-_{\vec{k}} \hat{a}^-_{-\vec{k}})$$
(19.183)

up to terms with 4 creation/annihilation operators, which are of order n'^2 where

$$n' = \frac{N - N_0}{V} = density \ of \ particles \ not \ in \ condensate$$
(19.184)

We make the approximation of neglecting these anharmonic terms, which is good for $n' \ll n$.

The remaining Hamiltonian is a quadratic form which we need to diagonalize to solve the problem.

We use the so-called Bogoliubov transformation. We assume that

$$\hat{a}_{\vec{k}} = u_{\vec{k}}\hat{\alpha}_{\vec{k}} + v_{\vec{k}}\hat{\alpha}_{-\vec{k}}^{+} \quad , \quad \hat{a}_{\vec{k}}^{+} = u_{\vec{k}}\hat{\alpha}_{\vec{k}}^{+} + v_{\vec{k}}\hat{\alpha}_{-\vec{k}}$$
(19.185)

with real coefficients. We then require that the operators $\hat{\alpha}$ satisfy Bose commutation relations

$$\left[\hat{\alpha}_{\vec{k}}, \hat{\alpha}_{\vec{k}'}\right] = \left[\hat{\alpha}_{\vec{k}}^+, \hat{\alpha}_{\vec{k}'}^+\right] = 0 \quad , \quad \left[\hat{\alpha}_{\vec{k}}, \hat{\alpha}_{\vec{k}'}^+\right] = \delta_{\vec{k}\vec{k}'} \tag{19.186}$$

This requires that $u_{\vec{k}}^2 - v_{\vec{k}}^2 = 1.$ The inverse transformations are

$$\hat{\alpha}_{\vec{k}} = u_{\vec{k}} \hat{a}_{\vec{k}} - v_{\vec{k}} \hat{a}_{-\vec{k}}^+ \quad , \quad \hat{\alpha}_{\vec{k}}^+ = u_{\vec{k}} \hat{a}_{\vec{k}}^+ - v_{\vec{k}} \hat{a}_{-\vec{k}} \tag{19.187}$$

We also have that

$$\hat{a}_{\vec{k}}^{+} \hat{a}_{\vec{k}} = u_{\vec{k}}^{2} \alpha_{\vec{k}}^{+} \alpha_{\vec{k}} + v_{\vec{k}}^{2} \alpha_{-\vec{k}} \alpha_{-\vec{k}}^{+} + u_{\vec{k}} v_{\vec{k}} (\alpha_{\vec{k}}^{+} \alpha_{-\vec{k}}^{+} + \alpha_{\vec{k}} \alpha_{-\vec{k}}) \hat{a}_{\vec{k}}^{+} \hat{a}_{-\vec{k}}^{+} = u_{\vec{k}}^{2} \alpha_{\vec{k}}^{+} \alpha_{-\vec{k}}^{+} + v_{\vec{k}}^{2} \alpha_{\vec{k}} \alpha_{-\vec{k}} + u_{\vec{k}} v_{\vec{k}} (\alpha_{\vec{k}}^{+} \alpha_{\vec{k}} + \alpha_{-\vec{k}} \alpha_{-\vec{k}}^{+}) \hat{a}_{\vec{k}} \hat{a}_{-\vec{k}} = u_{\vec{k}}^{2} \alpha_{\vec{k}} \alpha_{-\vec{k}} + v_{\vec{k}}^{2} \alpha_{\vec{k}}^{+} \alpha_{-\vec{k}}^{+} + u_{\vec{k}} v_{\vec{k}} (\alpha_{-\vec{k}}^{+} \alpha_{-\vec{k}} + \alpha_{\vec{k}} \alpha_{\vec{k}}^{+})$$

The Hamiltonian becomes

$$\begin{split} \hat{H} &= \frac{1}{2V} N^2 V_0 \\ &+ \sum_{\vec{k} \neq 0} \left(\frac{\hbar^2 k^2}{2m} + n V_{\vec{k}} \right) \left[u_{\vec{k}}^2 \alpha_{\vec{k}}^+ \alpha_{\vec{k}} + v_{\vec{k}}^2 \alpha_{\vec{k}} \alpha_{\vec{k}}^+ + u_{\vec{k}} v_{\vec{k}} (\alpha_{\vec{k}}^+ \alpha_{-\vec{k}}^+ + \alpha_{\vec{k}} \alpha_{-\vec{k}}) \right] \\ &+ \frac{N}{2V} \sum_{\vec{k} \neq 0} V_{\vec{k}} \left[(u_{\vec{k}}^2 + v_{\vec{k}}^2) (\alpha_{\vec{k}}^+ \alpha_{-\vec{k}}^+ + \alpha_{\vec{k}} \alpha_{-\vec{k}}) + 2u_{\vec{k}} v_{\vec{k}} (\alpha_{\vec{k}}^+ \alpha_{\vec{k}} + \alpha_{\vec{k}} \alpha_{\vec{k}}^+) \right] \end{split}$$
(19.188)

In order for the non-diagonal terms to vanish, we must have

$$\left(\frac{\hbar^2 k^2}{2m} + nV_{\vec{k}}\right) u_{\vec{k}} v_{\vec{k}} + \frac{N}{V} V_{\vec{k}} \left(u_{\vec{k}}^2 + v_{\vec{k}}^2\right) = 0$$
(19.189)

This equation together with $u_{\vec{k}}^2-v_{\vec{k}}^2=1$ is sufficient to determine $u_{\vec{k}}^2$ and $v_{\vec{k}}^2.$ If we define

$$h\omega_{\vec{k}} = \left[\left(\frac{\hbar^2 k^2}{2m} + nV_{\vec{k}} \right)^2 - \left(nV_{\vec{k}} \right)^2 \right]^{1/2} \\ = \left[\left(\frac{\hbar^2 k^2}{2m} \right)^2 + \frac{nk^2 V_{\vec{k}}}{m} \right]^{1/2}$$
(19.190)

then we get

$$u_{\vec{k}}^{2} = \frac{\hbar\omega_{\vec{k}} + \left(\frac{\hbar^{2}k^{2}}{2m} + nV_{\vec{k}}\right)}{2\hbar\omega_{\vec{k}}} \quad , \quad v_{\vec{k}}^{2} = \frac{-\hbar\omega_{\vec{k}} + \left(\frac{\hbar^{2}k^{2}}{2m} + nV_{\vec{k}}\right)}{2\hbar\omega_{\vec{k}}} \tag{19.191}$$

and

$$u_{\vec{k}}v_{\vec{k}} = -\frac{nV_{\vec{k}}}{2\hbar\omega_{\vec{k}}} \quad , \quad v_{\vec{k}}^2 = \frac{\left(nV_{\vec{k}}\right)^2}{2\hbar\omega_{\vec{k}}\left(\hbar\omega_{\vec{k}} + \frac{\hbar^2k^2}{2m} + nV_{\vec{k}}\right)} \tag{19.192}$$

Finally, the Hamiltonian becomes

$$\hat{H} = \frac{1}{2V}N^2 V_0 - \frac{1}{2}\sum_{\vec{k}\neq 0} \left(\frac{\hbar^2 k^2}{2m} + nV_{\vec{k}} - \hbar\omega_{\vec{k}}\right) + \sum_{\vec{k}\neq 0} \hbar\omega_{\vec{k}}\alpha^+_{\vec{k}}\alpha_{\vec{k}}$$
(19.193)

where

$$\frac{1}{2V}N^2V_0 - \frac{1}{2}\sum_{\vec{k}\neq 0} \left(\frac{\hbar^2k^2}{2m} + nV_{\vec{k}} - \hbar\omega_{\vec{k}}\right) = \text{ ground state energy } E_0 \qquad (19.194)$$

$$\sum_{\vec{k}\neq 0} \hbar \omega_{\vec{k}} \alpha_{\vec{k}}^{+} \alpha_{\vec{k}} = \text{ sum of oscillators or excitations}$$
(19.195)

The excitations (oscillators) or quanta that are created by the $\alpha^+_{\vec{k}}$ are called quasiparticles.

All the excited states correspond to different numbers of noninteracting bosons where each boson has the excitation energy

$$E_{\vec{k}} = \hbar\omega_{\vec{k}} = \left[\left(\frac{\hbar^2 k^2}{2m} + nV_{\vec{k}} \right)^2 - \left(nV_{\vec{k}} \right)^2 \right]^{1/2} \\ = \left[\left(\frac{\hbar^2 k^2}{2m} \right)^2 + \frac{nk^2 V_{\vec{k}}}{m} \right]^{1/2}$$
(19.196)

Quasiparticles appear in all kinds of physical systems at all energy scales.

The ground state of the system $|0\rangle$ is fixed by the condition that *no quasiparticles* are excited,

$$\alpha_{\vec{k}} \left| 0 \right\rangle = 0 \text{ for all } \vec{k} \tag{19.197}$$

The number of particles outside the condensate(the ground state) is given by

$$N' = \langle 0 | \sum_{\vec{k} \neq 0} \hat{a}^{+}_{\vec{k}} \hat{a}_{\vec{k}} | 0 \rangle = \langle 0 | \sum_{\vec{k} \neq 0} \hat{\alpha}_{\vec{k}} \hat{\alpha}^{+}_{\vec{k}} | 0 \rangle = \sum_{\vec{k} \neq 0} v_{\vec{k}}^{2}$$
(19.198)

For small $|\vec{k}|$ we have

$$E_{\vec{k}} = \hbar \omega_{\vec{k}} \approx c_s \hbar k \tag{19.199}$$

where

$$c_s = \sqrt{\frac{nV_0}{m}} = \text{speed of sound in fluid}$$
 (19.200)

This says that the long wavelength excitations have a linear dispersion relation (E versus k).

For large $|\vec{k}|$ we have

$$E_{\vec{k}} = \hbar\omega_{\vec{k}} = \frac{\hbar^2 k^2}{2m} + nV_{\vec{k}}$$
(19.201)

This corresponds to the dispersion relation for free particles whose energy is shifted by a mean potential $nV_{\vec{k}}$.

We can now understand qualitatively how superfluidity comes about.

Consider a small particle(call it a cluster) which could be several dirt atoms or a piece of a surrounding wall moving through a quantum liquid with the dispersion relations just described for the quasiparticle excitations, i.e., the quasiparticle energy rises linearly with k at low k and quadratically with k at large k.

The cluster can lose energy (experience friction) only by causing excitations in the fluid. For T > 0, there are already excitations present in the fluid at which the cluster may scatter and thus lose energy, but at T = 0, this is not the case. Let the initial momentum of the cluster be $\hbar \vec{q}$ and the momentum of the excitations be $\hbar \vec{k}$. In a scattering event of the cluster with the fluid, energy and momentum are conserved.

$$h\vec{q} = h\vec{q}' + h\vec{k}$$
, $\frac{\hbar^2 q^2}{2m} = \frac{\hbar^2 q'^2}{2m} + E(k)$ (19.202)

where $\hbar \vec{q}'$ is the momentum of the cluster after the scattering. The elementary excitations of the fluid (quasiparticles) are given by

$$E_{\vec{k}} = \hbar\omega_{\vec{k}} = \left[\left(\frac{\hbar^2 k^2}{2m} \right)^2 + \frac{nk^2 V_{\vec{k}}}{m} \right]^{1/2}$$
(19.203)

Consider the energy conservation equation. We have

$$\frac{\hbar^2 q^2}{2m} = \frac{\hbar^2 (\vec{q} - \vec{k})^2}{2m} + E(k)$$
(19.204)

or

$$0 = -\frac{\hbar^2}{2m}\vec{q}\cdot\vec{k} + \frac{\hbar^2k^2}{2m} + E(k)$$
(19.205)

This says that (let α be the angle between \vec{q} and \vec{k})

$$\cos \alpha = \frac{1}{v} \frac{E(k)}{\hbar k} + \frac{1}{v} \frac{\hbar k}{2m} + E(k)$$
(19.206)

where

$$v = \frac{hq}{m}$$
 = initial velocity of the cluster (19.207)

Now for the quasiparticle excitations

$$\frac{E(k)}{\hbar k} > c_s \tag{19.208}$$

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therefore, for the excitation (emission) of a quasiparticle the cluster velocity must be larger than c_s , i.e., $v > c_s$. This follows from the above relation as $k \to 0$ or the angle α becomes imaginary!

A cluster moving with $v < v_{critical} = c_s$ (in this model) cannot lose energy to the fluid. Thus, there is no friction and one has superfluidity. For liquid helium $v_{critical} << c_s$ and the physics is even more dramatic.

19.8 Spontaneous Symmetry Breaking in Quantum Mechanics

In quantum mechanics symmetry has a much more powerful role than in classical mechanics. Translational invariance in a classical system causes momentum to be conserved; in quantum mechanics it immediately implies that all eigenstates of the Hamiltonian are spread out with equal amplitude over all of space. It could be argued that because a chair is built of many microscopic particles that all obey the rules of quantum mechanics, the chair as a whole should also respect the symmetry of its Hamiltonian and be spread out over all of space. Clearly this situation is not physically realized. The way out of the seeming paradox is the spontaneous symmetry breaking of the collective system. The description of spontaneous symmetry breaking in macroscopic systems that are constructed from microscopic, quantum mechanical constituents is one of the highlights of condensed matter theory. It is used to explain the classical features of macroscopic systems ranging from crystals and antiferromagnets to superconductors.

The general idea behind spontaneous symmetry breaking is easily formulated: as a collection of quantum particles becomes larger, the symmetry of the system as a whole becomes more unstable against small perturbations. In the limit of an infinite system an infinitesimal perturbation is enough to cause the system to break the underlying symmetry of the Hamiltonian. The fact that the symmetry breaking can happen spontaneously is signaled by a set of noncommuting limits: In the complete absence of perturbations even a macroscopic system should conform to the symmetry of the Hamiltonian. However, in the presence of an infinitesimal perturbation a macroscopic system will be able to break the symmetry and end up in a classical state. This intuitive picture of spontaneous symmetry breaking is not always easy to demonstrate in an equally clear mathematical description of the process.

In this section we present a simple mathematical procedure that can be applied to the spontaneous breaking of any continuous symmetry and that naturally emphasizes the roles of the key players (the symmetry-breaking field, the thermodynamic limit, and the global excitations of a *thin spectrum*) in this symmetry breaking. The procedure is described by considering the example of a quantum harmonic crystal that spontaneously breaks translational symmetry. All of the methods, that is, bosonization, using the Bogoliubov transformation to identify the *thin spectrum* of states involved in spontaneous symmetry breaking, introducing a symmetry-breaking field in the collective dynamics, and considering a noncommuting order of limits, can be applied to other systems as well.

19.8.1 The Harmonic Crystal

As a basic example of spontaneous symmetry breaking, we consider how translational symmetry is broken in a crystalline lattice. Consider a harmonic crystal with the Hamiltonian

$$H = \sum_{j} \frac{p_{j}^{2}}{2m} + \frac{\kappa}{2} \sum_{j} (x_{j} - x_{j+1})^{2}$$
(19.209)

where j labels the N atoms in the lattice, which have mass m, momentum p_j , and position x_j . We consider here only a one- dimensional chain of atoms, but all of the following can be straightforwardly generalized to higher dimensions. The parameter κ gives the strength of the harmonic potential between neighboring atoms. The results on spontaneous symmetry breaking that follow are equally valid for anharmonic potentials.

In the standard treatment of the harmonic oscillator a Fourier transformation of the Hamiltonian is used to identify its eigenstates. We follow a slightly longer route by introducing boson (phonon) operators from the outset and diagonalizing them using the Bogoliubov transformation. This approach has the advantages that it naturally brings to the fore the *thin spectrum* of the crystal and enables us to keep track of the center of mass motion of the crystal as a whole. The momentum and position operators can be expressed in terms of boson operators as

$$p_j = iC\sqrt{\frac{\hbar}{2}} \left(b_j^+ - b_j \right) \quad , \quad x_j = \frac{1}{C}\sqrt{\frac{\hbar}{2}} \left(b_j^+ + b_j \right)$$
(19.210)

so that the commutation relation $[x_j, p_k] = i\hbar\delta_{jk}$ is satisfied. We choose $C^2 = \sqrt{2m\kappa}$ so that the Hamiltonian reduces to

$$H = \frac{\hbar}{4} \sqrt{\frac{2\kappa}{m}} \sum_{k} \left[2\left(b_{j}^{+}b_{j} + b_{j}b_{j}^{+}\right) - \left(b_{j}^{+} + b_{j}\right)\left(b_{j+1}^{+} + b_{j+1}\right) \right]$$
(19.211)

After a Fourier transformation we have

$$H = \sqrt{\frac{\hbar^2 \kappa}{2m}} \sum_{k} \left[A_k b_k^+ b_k + \frac{B_k}{2} \left(b_k^+ b_{-k}^+ + b_k b_{-k} \right) + 1 \right]$$
(19.212)

where $A_k = 2 - \cos(ka)$, $B_k = -\cos(ka)$, and *a* is the lattice constant. This Hamiltonian is still not diagonal, because the terms $b_k^+ b_{-k}^+$ and $b_k b_{-k}$ create

and annihilate two bosons at the same time. We get rid of these terms by introducing Bogoliubov transformed operators $\beta_k = \cosh(u_k)b_k + \sinh(u_k)b_k^+$ and choosing u_k such that the resulting Hamiltonian is diagonal. After this Bogoliubov transformation, the Hamiltonian in terms of transformed bosons is given by

$$H = \hbar \sqrt{\frac{\kappa}{m}} \sum_{k} \left[2\sin\left|\frac{ka}{2}\right| \left(\beta_{k}^{+}\beta_{k} + \frac{1}{2}\right) + \frac{\sqrt{2}}{4}\cos\left(ka\right) \right]$$
$$= 2\hbar \sqrt{\frac{\kappa}{m}} \sum_{k} \sin\left|\frac{ka}{2}\right| \left[n_{k} + \frac{1}{2}\right]$$
(19.213)

because $\sum_k \cos k = (N/2\pi) \int_{-\pi}^{\pi} dk \cos k = 0.$

19.8.2 The Thin Spectrum

The form Eq. (5) of the Hamiltonian in terms of phonon operators coincides with the standard textbook result. The use of the Bogoliubov transformation to obtain Eq. (5) has the advantage that it draws attention to a rather subtle point. When $k \to 0$ the excitation energy $\omega_k \to 0$, and the two parameters in the Bogoliubov transformation diverge $[\sinh(u_k) \to \infty \text{ and } \cosh(u_k) \to \infty$. This at k = 0 the canonical transformation is no longer well defined, and we should treat the k = 0 part of the Hamiltonian Eq. (1) separately from the rest. The excitations with k = 0 are the ones that describe the collective dynamics of the crystal as a whole, and therefore they are also the states that are involved in the collective symmetry breaking. The k = 0 part of the Hamiltonian, writ- ten in terms of the original operators, is given by

$$H_{coll} = \frac{p_{tot}^2}{2Nm} + \text{ constant}$$
(19.214)

where $p_{tot} = \sqrt{N}p_{k=0}$ is the total momentum of the system. It can easily be checked that this part of the Hamiltonian, which describes the external dynamics of the crystal as a whole, commutes with the rest of the Hamiltonian, which describes the internal dynamics of the phonon modes inside the crystal. We therefore focus on the collective part of the Hamiltonian and disregard the phonon spectrum given by Eq. (5).

Notice that by considering only the collective part of the Hamiltonian, we have effectively reduced the problem to a single-particle problem. The single particle in Eq. (6) with mass Nm and momentum p_{tot} describes the dynamics of the crystal as a whole. Its momentum and position are the center of mass momentum and position of the crystal. In contrast, Eq. (5) describes the internal degrees of freedom of the crystal and includes all many-body effects that arise from the coupling of the N individual atoms.

The relevant eigenstates of the collective Hamiltonian Eq. (6) are very low in

energy: their excitation energies scale as 1/n, where N is the number of atoms in the crystal. In the thermodynamic limit all of these states thus become nearly degenerate. Because of this property a combination of these states that break the symmetry of the Hamiltonian can be spontaneously formed in the thermodynamic limit. At the same time, these collective eigenstates are so few in number and of such low energy that their contribution to the free energy completely disappears in the thermodynamic limit. This vanishing contribution can be seen by looking at their contribution to the partition function.

Digression on the Partition Function

In statistical mechanics, the partition function Z is an important quantity that encodes the statistical properties of a system in thermodynamic equilibrium. It is a function of temperature and other parameters, such as the volume enclosing a gas. Most of the aggregate thermodynamic variables of the system, such as the total energy, free energy, entropy, and pressure, can be expressed in terms of the partition function or its derivatives.

There are actually several different types of partition functions, each corresponding to different types of statistical ensemble (or, equivalently, different types of free energy.) The canonical partition function applies to a canonical ensemble, in which the system is allowed to exchange heat with the environment at fixed temperature, volume, and number of particles. The grand canonical partition function applies to a grand canonical ensemble, in which the system can exchange both heat and particles with the environment, at fixed temperature, volume, and chemical potential. Other types of partition functions can be defined for different circumstances; see partition function (mathematics) for generalizations.

Canonical Partition Function - Definition

As a beginning assumption, assume that a thermodynamically large system is in constant thermal contact with the environment, with a temperature T, and both the volume of the system and the number of constituent particles fixed. This kind of system is called a canonical ensemble. Let us label with s (s = 1, 2, 3, ...) the exact states (microstates) that the system can occupy, and denote the total energy of the system when it is in microstate s as Es. Generally, these microstates can be regarded as discrete quantum states of the system.

The canonical partition function is

$$Z = \sum_{s} e^{-\beta E}$$

where the *inverse temperature* β is conveniently defined as

$$\beta = \frac{1}{k_B T}$$

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where k_B denotes Boltzmann's constant.

In quantum mechanics, the partition function can be more formally written as a trace over the state space (which is independent of the choice of basis):

$$Z = Tr\left(e^{-\beta H}\right)$$

where H is the quantum Hamiltonian operator. The exponential of an operator can be defined using the exponential power series.

Meaning and Significance

It may not be obvious why the partition function, as we have defined it above, is an important quantity. Firstly, let us consider what goes into it. The partition function is a function of the temperature T and the microstate energies E_1 , E_2 , E_3 , etc. The microstate energies are determined by other thermodynamic variables, such as the number of particles and the volume, as well as microscopic quantities like the mass of the constituent particles. This dependence on microscopic variables is the central point of statistical mechanics. With a model of the microscopic constituents of a system, one can calculate the microstate energies, and thus the partition function, which will then allow us to calculate all the other thermodynamic properties of the system.

The partition function can be related to thermodynamic properties because it has a very important statistical meaning. The probability P_s that the system occupies microstate s is

$$P_s = \frac{1}{Z} e^{-\beta E_s}$$

The partition function thus plays the role of a normalizing constant (note that it *does not* depend on s), ensuring that the probabilities sum up to one:

$$\sum_{s} P_s = \frac{1}{Z} \sum_{s} e^{-\beta E_s} = \frac{1}{Z} Z = 1$$

This is the reason for calling Z the *partition function*: it encodes how the probabilities are partitioned among the different microstates, based on their individual energies.

Calculating the Thermodynamics Total Energy

In order to demonstrate the usefulness of the partition function, let us calculate the thermodynamic value of the total energy. This is simply the expected value, or ensemble average for the energy, which is the sum of the microstate energies weighted by their probabilities:

$$\langle E \rangle = \sum_{s} E_{s} P_{s} = \frac{1}{Z} \sum_{s} E_{s} e^{-\beta E_{s}} = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial \beta}$$

or, equivalently,

$$\langle E \rangle = k_B T^2 \partial \ln Z \partial T$$

Incidentally, one should note that if the microstate energies depend on a parameter λ in the manner

$$E_s = E_s^{(0)} + \lambda A_s$$
 for all s

then the expected value of A is

$$\langle A \rangle = \sum_{s} A_{s} P_{s} = -\frac{1}{\beta} \frac{\partial}{\partial \lambda} \ln Z(\beta, \lambda)$$

This provides us with a method for calculating the expected values of many microscopic quantities. We add the quantity artificially to the microstate energies (or, in the language of quantum mechanics, to the Hamiltonian), calculate the new partition function and expected value, and then set λ to zero in the final expression.

Relation to Thermodynamic Variables

We now state the relationships between the partition function and the various thermodynamic parameters of the system. These results can be derived using the method of the previous section and the various thermodynamic relations. As we have already seen, the thermodynamic energy is

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta}$$

The variance in the energy (or *energy fluctuation*) is

$$\langle (\Delta E)^2 \rangle = \langle (E - \langle E \rangle)^2 \rangle = \frac{\partial^2 \ln Z}{\partial \beta^2}$$

The heat capacity is

$$C_v = \frac{\partial \langle E \rangle}{\partial T} = frac 1 k_B T^2 \langle (\Delta E)^2 \rangle$$

The entropy is

$$S = -k_B \sum_{s} P_s \ln P_s = k_B \left(\ln Z + \beta \langle E \rangle \right) = \frac{\partial}{\partial T} \left(k_B T \ln Z \right) = -\frac{\partial F}{\partial T}$$

where F is the Helmholtz free energy defined as F = U - TS, where $U = \langle E \rangle$ is the total energy and S is the entropy, so that

$$F = \langle E \rangle - TS = -k_B T \ln Z$$

Returning to our discussion. We have

$$Z_{thin} = \sum e^{-\beta H_{coll}} \propto \sqrt{N}$$

$$F_{thin} = -k_B T \ln (Z_{thin}) \propto \ln (N)$$
(19.215)

The free energy of the total system is an extensive quantity, so that $F_{thin}/F_{tot} \propto \ln{(N)}/N$ disappears in the limit $N \to \infty$, which is the so-called *thermodynamic limit*. The states of this part of the spectrum are thus invisible in thermodynamically measurable quantities such as for instance the specific heat of macroscopic crystals, and it is consequently called the *thin spectrum* of the quantum crystal.

To see how the states in the thin spectrum can conspire to break the translational symmetry, we need to add a small symmetry-breaking field to the Hamiltonian:

$$H_{coll}^{SB} = \frac{p_{tot}^2}{2Nm} + \frac{B}{2}x_{tot}^2$$
(19.216)

Here the symmetry-breaking field B is introduced as a mathematical tool and need not actually exist. We will send the value of B to zero at the end of the calculation. The Hamiltonian Eq. (8) is the standard form of the Hamiltonian for a quantum harmonic oscillator, and its eigenstates are well known. The ground state wavefunction can be written as

$$\psi_0(x_{tot}) = \left(\frac{m\omega N}{\pi\hbar}\right)^{1/4} e^{-(m\omega N/2\hbar)x_{tot}^2}$$
(19.217)

where $\omega = \sqrt{B/mN}$. This ground state is a wavepacket of the total momentum states that make up the thin spectrum. Apart from the ground state configuration there are also collective eigenstates that are described by the excitations of the harmonic oscillator Eq. (8). These excitations describe the collective motion of the crystal as a whole. As N becomes larger, the ground state wavepacket becomes more and more localized at the position $x_{tot} = 0$, until it is completely localized as $N \to \infty$. That this localization can occur spontaneously without the existence of a physical symmetry-breaking field B can be seen by considering the noncommuting limits

$$\lim_{N \to \infty} \lim_{B \to 0} |\psi_0(x_{tot})|^2 = \text{ constant}$$
(19.218)

$$\lim_{B \to 0} \lim_{N \to \infty} |\psi_0(x_{tot})|^2 = \delta(x_{tot})$$
(19.219)

If we do not include any symmetry-breaking field, then the crystal is always completely delocalized and respects the symmetry of the Hamiltonian. If we do allow for a symmetry-breaking field, then it turns out that in the limit of having infinitely many constituent particles, an infinitesimally small symmetry-breaking field is enough to completely localize the crystal at a single position. This mathematical instability implies that the symmetry breaking happens spontaneously in the thermodynamic limit(spontaneous symmetry breaking). Notice that once the crystal has been localized at a specific position and the unphysical symmetry-breaking field has been sent to zero, the delocalization of the crystal due to the spreading of its wavefunction will take a time proportional to N and can thus never be observed.

To see more rigorously whether or not the crystal as a whole is localized, we should look at the spatial fluctuations $\langle x_{tot}^2 \rangle$. The absolute size of these fluctuations by itself is meaningless. Their size becomes meaningful only if it is compared to the size of the crystal. Because the size of the crystal is proportional to the number of particles in the system, the appropriate order parameter in this case is of the crystal $\langle x_{tot}^2 \rangle / N$. This order parameter has a noncommuting order of limits as

$$\lim_{N \to \infty} \lim_{B \to 0} \langle x_{tot}^2 \rangle / N = \infty$$
(19.220)

$$\lim_{B \to 0} \lim_{N \to \infty} \langle x_{tot}^2 \rangle / N = 0 \tag{19.221}$$

which again signals the spontaneous localization of the crystal as a whole.

19.8.3 Subtleties

In the derivation of the spontaneous symmetry breaking of a harmonic crystal we have been somewhat sloppy in the definition of the symmetry-breaking field. After all, the collective model of Eq.(6) was only the k = 0 part of the full blown Hamiltonian in Eq. (1), but we did not consider the symmetry-breaking field to be only the k = 0 part of some other field acting on all atoms individually. It would therefore be better to start with a microscopic model, which already includes a symmetry-breaking field such as

$$H^{SB} = \sum_{j} \left[\frac{p_j^2}{2m} + \frac{\kappa}{2} (x_j - x_{j+1})^2 + B(1 - \cos(x_j)) \right]$$
(19.222)

$$\rightarrow H_{coll}^{SB} \approx \frac{p_{tot}^2}{2Nm} + \frac{B}{2N} x_{tot}^2$$
(19.223)

In Eq. (15) we again consider only the k = 0 part of the Hamiltonian and have expanded the cosine to quadratic order. The fact that the symmetrybreaking field now scales as 1/N is a direct consequence of our definition of the microscopic symmetry-breaking field. The factor 1/N cannot be avoided if we insist that the microscopic Hamiltonian be extensive. This factor might seem to imply an end to the localization of the total wavefunction $\psi_0(x_{tot})$, but spontaneous symmetry breaking is still possible as long as we consider the correct order parameter. Even though the wavefunction itself does not reduce to a Dirac delta function anymore, the spatial fluctuations of the crystal compared to its size still become negligible in the thermodynamic limit if an infinitesimal symmetry-breaking field is included:

$$\lim_{N \to \infty} \lim_{B \to 0} \langle x_{tot}^2 \rangle / N = \infty$$
(19.224)

$$\lim_{B \to 0} \lim_{N \to \infty} \langle x_{tot}^2 \rangle / N = 0$$
(19.225)

Once again the disappearance of fluctuations in the thermodynamic limit signals the spontaneous localization of the crystal as a whole.

This digression into extensivity and the correct choice for the symmetry-breaking field seems unnecessary for understanding the essential ingredients of spontaneous symmetry breaking, and therefore we have ignored these subtleties in our main treatment of quantum spontaneous symmetry breaking. In the application of this procedure to other systems, such as antiferromagnets and superconductors, these issues don't arise because we are forced to consider extensive models from the outset. In these cases, however, the mathematics of diagonalizing the collective Hamiltonian is a bit more involved.

Summarizing, this section provides a simple way of explaining the appearance of spontaneous symmetry breaking in quantum systems. The procedure starts with the bosonization of the microscopic Hamiltonian. The quadratic part of the bosonized Hamiltonian can in principle be diagonalized using a Bogoliubov transformation, but in doing so we find that there are some modes for which the transformation is ill-defined. These singular modes are the ones that describe the dynamics of the system as a whole (in contrast to the dynamics of constituent particles within the system). These collective excitations should be treated separately from all other modes, and together they define the collective part of the Hamiltonian of the system. The eigenstates of this collective Hamiltonian that scale as 1/N form the thin spectrum. It is a combination of these states that make up the symmetry broken wavefunction. As a mathematical tool necessary to be able to see the symmetry breaking explicitly, we introduced the symmetry-breaking field B. If we look at the new ground state wavefunction or at a suitably defined order parameter for the system, we see that in the thermodynamic limit an infinitesimally small field B is enough to completely break the symmetry of the underlying Hamiltonian. It is thus argued that symmetry breaking can happen spontaneously in the limit $N \to \infty$.

This method as presented can be adapted to describe rotors, antiferromagnets, and even superconductors, and should in principle be applicable to all quantum systems that spontaneously break some continuous symmetry.

19.9 Problems

19.9.1 Bogoliubov Transformations

Consider a Hamiltonian for Bosonic operators \hat{b}_k^+, \hat{b}_k of the form

$$\hat{H} = E(k)\hat{b}_{k}^{\dagger}\hat{b}_{k} + A(k)\left[\hat{b}_{k}^{\dagger}\hat{b}_{-k}^{\dagger} + \hat{b}_{k}\hat{b}_{-k}\right]$$

Define a Bogoliubov transformation to new Bosonic operators $\hat{\alpha}_k^+, \hat{\alpha}_k$ as follows:

 $\hat{b}_k = \cosh 2\theta_k \hat{\alpha}_k + \sinh 2\theta_k \hat{\alpha}_{-k}^+ \ , \ \hat{b}_k^+ = \cosh 2\theta_k \hat{\alpha}_k^+ + \sinh 2\theta_k \hat{\alpha}_{-k}$

(a) Assume that E(k), A(k), θ_K are all even functions of k and find the form of $\sinh 2\theta_k$ as a function of A(k), E(k) so that

$$\hat{H} = \Omega(k)\hat{\alpha}_k^+\hat{\alpha}_k + F(k)$$

and find $\Omega(k)$ and F(k).

- (b) Show that if $[\hat{b}_k^+, \hat{b}_k] = 1$, $[\hat{b}_k, \hat{b}_k] = [\hat{b}_k^+, \hat{b}_k^+] = 0$, then $[\hat{\alpha}_k^+, \hat{\alpha}_k] = 1$, $[\hat{\alpha}_k, \hat{\alpha}_k] = [\hat{\alpha}_k^+, \hat{\alpha}_k^+] = 0$.
- (c) Show that if the operators \hat{b}_k^+, \hat{b}_k are Fermionic instead of Bosonic, the Bogoliubov transformation must have $\cosh \theta_k \to \cos \theta_k$ and $\sinh \theta_k \to \sin \theta_k$ so that the new operators $\hat{\alpha}_k^+, \hat{\alpha}_k$ now obey anticommutation rules.

19.9.2 Weakly Interacting Bose gas in the Bogoliubov Approximation

In this case we have the Hamiltonian

$$\hat{H} = \sum_{k} \varepsilon(k) \hat{a}_{k}^{\dagger} \hat{a}_{k} + \frac{1}{2V} \sum_{q} V_{q} \sum_{p,k} \hat{a}_{p+q}^{\dagger} \hat{a}_{k-q}^{\dagger} \hat{a}_{k} \hat{a}_{p}$$

Consider the operator $\hat{K} = \hat{H} - \mu \hat{N}$ where $\hat{N} = \sum_k \hat{a}_k^+ \hat{a}_k$. Define $\hat{a}_0 = \sqrt{N_0} e^{i\theta} + \hat{b}_0$, $\hat{a}_{k\neq 0} = \hat{b}_{k\neq 0}$.

- (a) Separate the terms of order N_0^2 , $N_0\sqrt{N_0}$, N_0 in the interaction term, show that these are quadratic in \hat{b}, \hat{b}^+ , and show that terms of order $\sqrt{N_0}$ and 1 are cubic and quartic in \hat{b}, \hat{b}^+ . Neglect the terms of $O(\sqrt{N_0})$ and O(1), which is the Bogoliubov approximation, and write down \hat{K} only keeping terms up to quadratic order in \hat{b}, \hat{b}^+ .
- (b) Show that in this Bogoliubov approximation that $\hat{K} = \hat{K}_Q + \hat{K}_{cl}$ where \hat{K}_Q is quadratic and linear in \hat{b}, \hat{b}^+ and \hat{K}_{cl} is purely classical and independent of \hat{b}, \hat{b}^+ . Establish a relation $\mu = \mu(N_0)$ by minimization of \hat{K}_{cl} , i.e.,

$$\left. \frac{\partial \hat{K}_{cl}}{\partial N_0} \right|_{\mu} = 0$$

This is the *Gross-Pitaevskii equation*. Show that imposing this condition leads to the cancellation of the terms linear in \hat{b}, \hat{b}^+ in \hat{K}_Q .

(c) Diagonalize the resulting quadratic form for \hat{K}_Q by a Bogoliubov transformation:

$$b_k^+ e^{i\theta} = \hat{c}_k \cosh \phi_k + \hat{c}_{-k}^+ \sinh \phi_k$$

Find $\cosh \phi_k$, $\sinh \phi_k$ by requesting the cancellation of terms $\hat{c}_k^+ \hat{c}_{-k}^+$, $\hat{c}_k \hat{c}_{-k}$. Show that in this Bogoliubov transformation,

$$\hat{K}_Q = \sum_k \hat{c}_k^+ \hat{c}_k \hbar \Omega(k) + K_0$$

Find $\Omega(k)$ and K_0 , consider $V_q = V_0$ constant and evaluate the integral for K_0 .

19.9.3 Problem 19.9.2 Continued

(a) Invert the Bogoliubov transformation in part (c) of Problem 19.9.2 and show that

$$\hat{c}_k = b_k \cosh \phi_k - b_{-k}^+ \sinh \phi_k$$

where $\tilde{b}_k = \hat{b}_k e^{-i\theta}$. Use

$$e^{A}Be^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \dots$$

to show that

$$\hat{c}_k = U(\phi)\tilde{b}_k U^{-1}(\phi)$$

where $U(\phi)$ is the unitary operator

$$U(\phi) = e^{\sum_{k>0} \phi_k \left(\tilde{b}_k^+ \tilde{b}_{-k}^+ - \tilde{b}_k \tilde{b}_{-k}\right)}$$

(b) Show that the ground state of K̂ in the Bogoliubov approximation is |GS⟩ = U(φ) |Õ⟩ where |Õ⟩ is the vacuum of the operators b̃_k : b̃_k |Õ⟩ = 0 for all k. Argue that |GS⟩ is a linear superposition of states with a pair of momenta k̄, -k̄ respectively. This is a squeezed quantum state (see Chapter 14 example). These states are ubiquitous in quantum optics and quantum controlled nanoscale systems.

19.9.4 Mean-Field Theory, Coherent States and the Grtoss-Pitaevkii Equation

Consider the pair potential $V(\vec{x} - \vec{y}) = V_0 \delta^3(\vec{x} - \vec{y})$ and introduce the coherent states of the Bosonic operator $|\psi(\vec{x})\rangle$ such that $\hat{\psi}(\vec{x})|\psi(\vec{x})\rangle = \psi(\vec{x})|\psi(\vec{x})\rangle$. Include a one-body *trap* potential in the Hamiltonian \hat{H} :

$$\begin{split} \hat{H} &= \int d^3 x \, \hat{\psi}^+(\vec{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} + U(\vec{x}) \right) \hat{\psi}(\vec{x}) \\ &+ \frac{1}{2} \int \int d^3 x \, d^3 y \, \hat{\psi}^+(\vec{x}) \hat{\psi}^+(\vec{y}) V(\vec{x} - \vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x}) \end{split}$$

(a) Minimize the energy $E(\psi) = \langle \psi | \hat{K} | \psi \rangle$ where $|\psi\rangle$ is the coherent state above with $\langle \psi | \psi \rangle = 1$ and show that

$$\frac{\partial E}{\partial \psi^*(\vec{x})} = 0$$

leads to the Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + U(\vec{x}) - \mu\right] \psi(\vec{x}) + V_0 |\psi(\vec{x})|^2 \psi(\vec{x}) = 0$$

with the constraint that $\int |\psi(\vec{x})|^2 d^3x = N$.

- (b) Define new operators ψ̂(x) → ψ(x) + η̂(x) where ψ(x) is the solution to the Gross-Pitaevskii equation and write K̂ up to quadratic order in η̂(x), η̂⁺(x). Show that terms linear in η̂(x), η̂⁺(x) are cancelled by ψ(x) being a solution to the Gross-Pitaevskii equation.
- (c) Introduce the Bogoliubov transformation:

$$\hat{\phi}(\vec{x}) = u(\vec{x})\hat{\eta}(\vec{x}) + v(\vec{x})\hat{\eta}^{+}(\vec{x}) , \quad \hat{\phi}^{+}(\vec{x}) = u^{*}(\vec{x})\hat{\eta}^{+}(\vec{x}) + v^{*}(\vec{x})\hat{\eta}(\vec{x})$$

Show that $[\hat{\phi}(\vec{x}), \hat{\phi}^+(\vec{y})] = \delta^3(\vec{x} - \vec{y})$ if $|u(\vec{x})|^2 + |v(\vec{x})|^2 = 1$.

(d) Write \hat{K} up to quadratic order in $\hat{\eta}, \hat{\eta}^+$ found in part (b) in terms of $\hat{\phi}, \hat{\phi}^+$. What is the equation that U, V must obey so that the terms of the form $\hat{\phi}^2, \hat{\phi}^{+2}$ are cancelled? These are the *Bogoliubov-DeGennes equations*!

19.9.5 Weakly Interacting Bose Gas

Consider a homogeneous, weakly interacting Bose gas with Hamiltonian

$$\hat{H} = \int d^3x \,\hat{\psi}^+(\vec{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\psi}(\vec{x}) + \int \int d^3x \, d^3y \,\hat{\psi}^+(\vec{x}) \hat{\psi}^+(\vec{y}) V(\vec{x} - \vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x})$$

(a) Consider $V(\vec{x} - \vec{y}) = -|V_0|\delta^3(\vec{x} - \vec{y})$ and assume a condensate with N_0 particles. Obtain the operator for $\hat{K} = \hat{H} - \mu \hat{N}$ in the Bogoliubov approximation. By a canonical Bogoliubov transformation bring it to the form

$$\hat{K} = \sum_{k} \hbar \Omega(k) \hat{c}_{k}^{\dagger} \hat{c}_{k} + K_{0}$$

Show that $\Omega(k)$ becomes imaginary for some values of $0 < k < k_{max}$.

(b) What is k_{max} ? What is the physical reason for this imaginary value and what do they mean?

19.9.6 Bose Coulomb Gas

Consider the same problem as Problem 19.9.1, but now with

$$V(\vec{x} - \vec{y}) = \frac{e^2}{|\vec{x} - \vec{y}|}$$
(19.226)

which is the Coulomb potential. Namely, consider a weakly interacting Bose ga of charged particles (and assume a homogeneous neutralizing background like in the so-called *Jellium* model).

- (a) Obtain the energy eigenvalues $\hbar\Omega(k)$ in the Bogoliubov approximation. Show that now $\lim_{k\to 0} \Omega(k) = \Omega(0) \neq 0$. What is $\Omega(0)$? Compare to the result for plasma oscillations in an electron gas.
- (b) Give the behavior of the Bogoliubov coefficients for small k. This is related to long-range behavior of the forces. Goldstone's theorem states that any theory with an exact symmetry other than that of the vacuum must contain a massless particle. Does this case violate Goldstone's theorem?

19.9.7 Pairing Theory of Superconductivity

The B(ardeen)C(ooper)S(chrieffer) Hamiltonian in the mean-field approximation is

$$\hat{K} = \hat{H} - \mu \hat{N} = \sum_{k} \varepsilon(k) \left(\hat{a}_{k\uparrow}^{\dagger} \hat{a}_{k\uparrow} + \hat{a}_{k\downarrow}^{\dagger} \hat{a}_{k\downarrow} \right) + \sum_{k} \left[\Delta \hat{a}_{k\uparrow}^{\dagger} \hat{a}_{-k\downarrow} + \Delta^{*} \hat{a}_{-k\downarrow}^{\dagger} \hat{a}_{k\uparrow} \right]$$

where $\hat{a}^+_{k\uparrow,\downarrow}$ are creation operators of an electron of spin up or down and momentum \vec{k} and

$$\Delta = -\frac{g}{V} \sum_{k'}^{\prime} \langle GS | \hat{a}_{-k\downarrow} \hat{a}_{k\uparrow} | GS \rangle$$

 $|GS\rangle$ is the ground state of \hat{K} and $\sum_{k'}$ is a sum over states with

$$0 \le \varepsilon(k') \le \hbar \omega_m$$
 and $\varepsilon(k') = \varepsilon(k) - \mu = \frac{\hbar^2 k^2}{2m} - \mu$

(a) Diagonalize \hat{K} by a Bogoliubov transformation, i.e., introduce new operators

$$\hat{A}_k = u_k \hat{a}_{k\uparrow} - v_k \hat{a}^+_{-k\downarrow} , \quad \hat{B}_k = v_k \hat{a}_{k\uparrow} + u_k \hat{a}^+_{-k\downarrow}$$

and their respective Hermitian conjugates with u_k, v_k and even in k. Show that the transformation is canonical, namely, that \hat{A}, \hat{B} obey the usual commutation relations if $u_k^2 + v_k^2 = 1$. It is convenient to write

$$u_k = \left[\frac{1}{2}(1+\alpha_k)\right]^{1/2}$$
, $v_k = -\left[\frac{1}{2}(1-\alpha_k)\right]^{1/2}$

Invert the Bogoliubov transformation and write \hat{K} in terms of $\hat{A}, \hat{A}^+, \hat{B}, \hat{B}^+$. Choose α_k so that \hat{K} becomes

$$\hat{K} = \sum_{k} E(k) \left[hat A_k^{\dagger} \hat{A}_k + \hat{B}_k^{\dagger} \hat{B}_k \right] + K_0$$

that is, choose α_k to make terms like $\hat{A}\hat{B}$ vanish. Find E(k).

(b) Obtain a self-consistent equation for Δ by evaluating $\langle GS | \hat{a}_{-k\downarrow} \hat{a}_{k\uparrow} | GS \rangle$ and solve this equation by replacing

$$\frac{1}{V}\sum_{k'}' \to \int_0^{\hbar\omega_m} N(\varepsilon) \, d\varepsilon$$

where $N(\varepsilon)$ is the density of states so that

$$N(\varepsilon)\,d\varepsilon = \frac{d^3k}{(2\pi)^3}$$

and assume that $N(\varepsilon) \approx N(0)$.

- (c) Obtain the distribution function $\langle GS | \hat{a}_{k\uparrow}^{\dagger} \hat{a}_{k\uparrow} | GS \rangle$
- (d) Show that $E(0) = \Delta =$ gap and evaluate the resulting integral in part (b) to give the gap Δ as a function of gN(0) for $gN(0) \ll 1$.

19.9.8 Second Quantization Stuff

1. Quantum Chain of Oscillators

Consider a chain of atoms with masses m connected by springs of rigidity γ :

$$H_{ph} = \sum_{n=-\infty}^{\infty} \left[\frac{p_n^2}{2m} + \frac{\gamma}{2} (u_n - u_{n+1})^2 \right]$$

where u_n are the displacements of atoms from their equilibrium positions, and p_n are the corresponding conjugate momenta.

Consider the problem in quantum mechanics, i.e., treat \hat{u}_n and \hat{p}_n as operators satisfying the canonical commutation relation $[\hat{p}_n, \hat{u}_{n'}] = -i\hbar\delta_{n,n'}$

Diagonalize the quantum Hamiltonian above. In order to do this, first do the Fourier transform: $\hat{u}_n \rightarrow \hat{u}_k$, $\hat{p}_n \rightarrow \hat{p}_k$ and then introduce the creation and annihilation operators of *phonons* \hat{a}_k^+ and \hat{a}_k by the following formula:

$$\hat{u}_k = \sqrt{\frac{\hbar}{2m\omega(k)}} (\hat{a}_k + \hat{a}_k^+) , \quad \hat{p}_k = -i\sqrt{\frac{\hbar m\omega(k)}{2}} (\hat{a}_k - \hat{a}_k^+)$$

Write the Hamiltonian in terms of \hat{a}_k^+ and \hat{a}_k and determine the phonon spectrum $\omega(k)$. Calculate the ground state energy of the system.

2. Interaction between Phonons

Suppose the springs have small anharmonicity γ' , so the Hamiltonian of the system has the additional term

$$H'_{ph} = \sum_{n=-\infty}^{\infty} \gamma' (u_n - u_{n+1})^3$$

Rewrite the Hamiltonian in terms of the phonon operators \hat{a}_k^+ and \hat{a}_k introduced in part (1). What can you say about momentum conservation of the phonons in the new Hamiltonian?

3. Electron-Phonon Interaction

Suppose electrons are also present on the same chain of atoms. Suppose that the electrons can make transitions between neighboring lattice sites with the probability amplitude t_n so that

$$H_{el} = \sum_{n=-\infty}^{\infty} t_n \hat{\psi}_{n+1}^+ \hat{\psi}_n + h.c.$$

where $\hat{\psi}_n^+$ and $\hat{\psi}_n$ are the fermion operators creating and annihilating electrons on the site n.

In the case $t_n = t = \text{constant}$, diagonalize the electron Hamiltonian by Fourier transform $\hat{\psi}_n \rightarrow \hat{\psi}_k$, and determine the spectrum $\varepsilon(k)$ of electronic excitations.

In general, the amplitude of electron tunneling t_n depends on the relative diosplacement of the nearest neighboring atoms $u_n - u_{n+1}$. Let us expand t_n as a function of $(u_n - u_{n+1})$ to the first order: $t_n = t + (u_n - u_{n+1})t'$. When substituted into the electron Hamiltonian, the second term gives the following Hamiltonian:

$$H_{el-ph} = t' \sum_{n=-\infty}^{\infty} (u_n - u_{n+1}) \hat{\psi}_{n+1}^+ \hat{\psi}_n + h.c$$

Rewrite this last Hamiltonian in terms of phonon and electron operators \hat{a}_k and $\hat{\psi}_k$ and their conjugates. Comment on conservation of momentum. This Hamiltonian describes the electron-phonon interaction. Phonons are excitations of the lattice or lattice vibrations.

19.9.9 Second Quantized Operators

Write down the second-quantized form of the following first-quantized operators describing N particles in both a position space basis $(\hat{\psi}(\vec{r}))$ and a momentum space basis (\hat{a}_k) :

- (a) particle density at \vec{r} : $\rho(\vec{r}) = \sum_{\ell} \delta(\vec{r} \vec{r}_{\ell})$
- (b) total number of particles: $\sum_{\ell} 1 = N$
- (c) charge current density at \vec{r} : $\vec{j}_e(\vec{r}) = \frac{e}{2m} \sum_{\ell} \left[\vec{p}_\ell \delta(\vec{r} \vec{r}_\ell) + \delta(\vec{r} \vec{r}_\ell) \vec{p}_\ell \right]$
- (d) magnetic moment density at \vec{r} : $\vec{m}(\vec{r}) = (g/2) \sum_{\ell} \vec{\sigma}_{\ell} \delta(\vec{r} \vec{r}_{\ell})$

19.9.10 Working out the details in Section 19.8

(1) Check that the thin spectrum of a harmonic crystal is indeed *thin*, that is,

- (a) Show that only the lowest \sqrt{N} total momentum states are not exponentially suppressed in the symmetry broken wavefunction (19.217). (This result implies that only the lowest \sqrt{N} total momentum states contribute to the symmetry broken wavefunction, and these states all become degenerate in the thermodynamic limit).
- (b) Calculate the partition function of the thin spectrum states and show that it scales as \sqrt{N} , so that the contribution of these states to the free energy vanishes in the thermodynamic limit.
- (2) Show the noncommutativity of the limits in Eq.(19.221) explicitly, by going through the following steps:
 - (a) Formulate the Hamiltonian of Eq.(19.216) in terms of the boson raising and lowering operators $b^+ = \sqrt{C/(2\hbar)}(x_{tot} (i/C)p_{tot})$ and $b = \sqrt{C/(2\hbar)}(x_{tot} + (i/C)p_{tot})$ where C is some constant.
 - (b) Choose C such that the Hamiltonian becomes diagonal and find its ground state.
 - (c) Evaluate the limits of Eq. (19.221) by expressing x_{tot}^2 in terms of boson operators and taking the expectation value with respect to the ground state of H_{coll}^{SB} .
- (3) Work out the Bogoliubov transformation of Eqs.(19.212) and (19.213) explicitly.
 - (a) Write the Hamiltonian of Eq. (19.212) in terms of the transformed bosons $\beta_k = \cosh(u_k)b_{-k} + \sinh(u_k)b_k^+$.
 - (b) Which value should be chosen for u_k in order for the Bogoliubov transformation to yield the diagonal Hamiltonian of Eq. (19.213) [Answer: $\tanh(2u_k) = B_k/A_k$].

Chapter 20

Relativistic Wave Equations

Electromagnetic Radiation in Matter

20.1 Spin 0 particles: Klein-Gordon Equation

A classical nonrelativistic free particle has an energy-momentum relation $E = p^2/2m$. Under a Galilean transformation to a new coordinate system traveling with $-\vec{v}$ with respect to the first system, we have

$$\vec{r}' = \vec{r} + \vec{v}t$$
 , $t' = t$ (20.1)

which gives

$$\vec{u}' = \frac{d\vec{r}'}{dt'} = \frac{d\vec{r}}{dt} + \vec{v} = \vec{u} + \vec{v}$$

$$m' = m$$

$$\vec{p}' = \vec{p} + m\vec{v}$$

We then have

$$\vec{F}' = \frac{d\vec{p}'}{dt'} = \frac{d\vec{p}}{dt} = \vec{F}$$
(20.2)

which implies the invariance of the form $E = p^2/2m$, i.e.,

$$E' = \int \vec{F}' \cdot d\vec{r}' = \frac{1}{m'} \int \vec{p}' \cdot d\vec{p}' = \frac{\vec{p}'^2}{2m'}$$
$$E = \int \vec{F} \cdot d\vec{r} = \frac{1}{m} \int \vec{p} \cdot d\vec{p} = \frac{\vec{p}^2}{2m}$$

and

$$E' = \frac{\vec{p}'^2}{2m'} = \frac{(\vec{p} + m\vec{v})^2}{2m} = E + \vec{p} \cdot \vec{v} + \frac{1}{2}mv^2$$
(20.3)

Thus, the final Galilean transformation relations are

$$E' = E + \vec{p} \cdot \vec{v} + \frac{1}{2}mv^2$$
, $\vec{p}' = \vec{p} + m\vec{v}$ (20.4)

which, as shown, leaves the quadratic form $E = p^2/2m$ invariant, i.e., if $E = \vec{p}^2/2m$, then $E' = \vec{p}'^2/2m'$ and we derive the transformation rules for E and \vec{p} from that condition.

The non-relativistic Schrodinger equation for the free particle then follows from the standard identifications

$$\begin{split} E &\to i\hbar \frac{\partial}{\partial t} \quad , \quad \vec{p} \to \frac{\hbar}{i} \nabla \\ H\psi &= E\psi \quad , \quad H = \frac{p^2}{2m} \end{split}$$

which gives

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi \tag{20.5}$$

It is clear from the form of the Schrodinger equation for a free particle that the equation cannot be invariant under Lorentz transformation (Lorentz covariant), i.e., the time derivative is first order and the space derivatives are second order.

20.1.1 How to find correct form of relativistic wave equation?

Before proceeding let us recall some results from special relativity. Components of spacetime four-vectors will be labeled by Greek indices and the components of spatial three-vectors will be labeled by Latin indices and we will use Einstein summation convention.

Starting from $x^{\mu}(s) = (ct, \vec{x}) = (x^0, \vec{x})$, the contravariant 4-vector representation of the worldline as a function of the proper time s, we first obtain the 4-velocity, i.e.,

$$\dot{x}^{\mu}(s) = \frac{dx^{\mu}(s)}{ds} = \frac{dx^{\mu}(s)}{\frac{1}{\gamma}dx^{0}} = \gamma\left(\frac{dx^{0}}{dx^{0}}, \frac{d\vec{x}}{dx^{0}}\right) = \gamma\left(1, \vec{v}/c\right)$$
(20.6)

where

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \quad , \quad \vec{v} = \frac{d\vec{x}}{dt} = c\frac{d\vec{x}}{dx^0}$$
(20.7)

The 4-momentum vector is then given by

$$p^{\mu} = mc\dot{x}^{\mu}(s) = \gamma m(c, \vec{v}) = (E/c, \vec{p})$$
(20.8)

where we have used the fact that

$$p^0 = \frac{E}{c} = \gamma m c$$
 , $m = \text{ rest mass}$ (20.9)

This says that the energy E and momentum \vec{p} transform as the components of a contravariant 4-vector and we know that the *square* of any 4-vector is invariant.

The metric tensor defined by

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$
(20.10)

allows the construction of the covariant components(using Einstein summation convention)

$$p_{\mu} = g_{\mu\nu}p^{\nu} = \left(\frac{E}{c}, -\vec{p}\right) \tag{20.11}$$

We can then calculate the invariant square or the invariant scalar product of the 4-momentum with itself as

$$p_{\mu}p^{\mu} = g_{\mu\nu}p^{\nu}p^{\mu} = \frac{E^2}{c^2} - \vec{p}^2 = m^2c^2$$
(20.12)

We therefore have the relativistic energy momentum relation

$$E = \left(\vec{p}^2 c^2 + m^2 c^4\right)^{1/2} \tag{20.13}$$

If we use this expression to construct a new wave equation by operator substitution we would have

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\hbar^2 c^2 \nabla^2 + m^2 c^4\right)^{1/2}\psi \qquad (20.14)$$

Although the energy formula is now relativistically correct, the time and space derivatives still do not appear symmetrically. In fact, a Taylor expansion of the square root gives infinitely high-order derivatives leading to a very difficult mathematical equation to deal with.

This fact, in itself, is not a valid reason for rejecting the equation.

There are, however, strong physical reasons for rejecting this equation. The equation says that the momentum space amplitude

$$\psi_{\vec{p}}(t) = \int d^3 r \, e^{-i\vec{p}\cdot\vec{r}/\hbar} \psi(\vec{r},t) \tag{20.15}$$

obeys the equation

$$i\hbar \frac{\partial \psi_{\vec{p}}(t)}{\partial t} = \left(p^2 c^2 + m^2 c^4\right)^{1/2} \psi_{\vec{p}}(t)$$
(20.16)

If we Fourier transform both sides back to position space we get

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \int d^3r' K(\vec{r}-\vec{r}\,')\psi(\vec{r}\,',t)$$
(20.17)

where

$$K(\vec{r} - \vec{r}') = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p} \cdot (\vec{r} - \vec{r}')/\hbar} \left(p^2 c^2 + m^2 c^4\right)^{1/2}$$
(20.18)

This equation for $\psi(\vec{r}, t)$ is *nonlocal*, which means that the value of the integral at *vecr* depends on the value of ψ at the other points *vecr'*. The function $K(\vec{r} - \vec{r}')$ is large as long as *vecr'* is within a distance

$$\approx \frac{h}{mc}$$
 = Compton wavelength (20.19)

from *vecr*. As a consequence of the nonlocality, the rate of change in time of ψ at the spacetime point (\vec{r}, t) depends on the values of ψ at points (\vec{r}', t) outside the light cone centered on (\vec{r}, t) .

If we construct a wave packet localized well within a Compton wavelength of the origin, then the packet will be nonzero an arbitrarily short time later at points as distant as the Compton wavelength.

Thus, this equation leads to violations of relativistic causality when used to describe particles localized to within more than a Compton wavelength, which is unacceptable.

Instead, we will start from an equation involving E^2 , i.e., we have

$$E^{2}\psi = \left(i\hbar\frac{\partial}{\partial t}\right)^{2}\psi = \left(\vec{p}^{2}c^{2} + m^{2}c^{4}\right)\psi = \left(-\hbar^{2}c^{2}\nabla^{2} + m^{2}c^{4}\right)\psi$$
$$\left(\nabla^{2} - \left(\frac{mc}{\hbar}\right)^{2}\right)\psi = \frac{1}{c^{2}}\frac{\partial^{2}\psi}{\partial^{2}t}$$
(20.20)

which looks like a classical wave equation with an extra term of the form

$$\left(\frac{mc}{\hbar}\right)^2 \tag{20.21}$$

It is called the *Klein-Gordon* equation. In 4-vector notation it looks like

$$\left(\partial_{\mu}\partial^{\mu} + \left(\frac{mc}{\hbar}\right)^{2}\right)\psi = 0 \quad , \quad \partial_{\mu} = \frac{\partial}{\partial x^{\mu}} \tag{20.22}$$

The equation can be generalized in a relativistically invariant way to include the coupling of charged particles to the electromagnetic field by the substitutions (corresponding to minimal coupling we discussed earlier in Chapter 8)

$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - e\Phi \quad , \quad \frac{\hbar}{i}\nabla \to \frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}$$
 (20.23)

to obtain

$$\frac{1}{c^2} \left(i\hbar \frac{\partial}{\partial t} - e\Phi(\vec{r}, t) \right)^2 \psi(\vec{r}, t) = \left(\left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}(\vec{r}, t) \right)^2 + m^2 c^2 \right) \psi(\vec{r}, t)$$
(20.24)

The Klein-Gordon equation has several unusual features.

First, it is second-order in time (space and time derivatives are now the same order). This means we need to specify twice as much initial information (the function and its derivative) at one time to specify the relativistic solution as compared to the nonrelativistic solution which only required specification of the function at one time.

This will mean that the equation has an extra degree of freedom. We will see shortly that this extra degree of freedom corresponds to specifying the *charge* of the particle and that the Klein-Gordon equation actually describes both a particle and its *antiparticle* together.

Second, since the equation is second order in time, the functions

$$\psi = e^{i(\vec{p}\cdot\vec{r} - Et)/\hbar} \tag{20.25}$$

satisfy the free particle equation with either sign of E, i.e.,

$$E = \pm \left(\vec{p}^2 c^2 + m^2 c^4\right)^{1/2} \tag{20.26}$$

The Klein-Gordon equation has negative energy solutions for a free particle! For these solutions when we *increase* the magnitude of the momentum \vec{p} , then the energy of the particle *decreases*! As we will see later, these negative energy solutions are real and will correspond to antiparticles, while the positive energy solutions will be particles.

In nonrelativistic Schrodinger theory we were able to interpret $\psi^*\psi$ as a positive probability density that was conserved in time (no sinks or sources of probability in nonrelativistic Schrodinger theory). Let us see what happens in the case of the Klein-Gordon equation.

For the Klein-Gordon equation

$$\int \psi^* \psi d^3 r \tag{20.27}$$

changes in time and thus, we cannot interpret $\psi^*(\vec{r},t)\psi(\vec{r},t)$ as being the probability of finding a particle at \vec{r} at time t.

We can, however, construct a different conserved density as follows. We write

$$\psi^* \left(\partial_\mu \partial^\mu + \left(\frac{mc}{\hbar} \right)^2 \right) \psi = 0 \tag{20.28}$$

and

$$\psi \left(\partial_{\mu} \partial^{\mu} + \left(\frac{mc}{\hbar} \right)^2 \right) \psi^* = 0 \tag{20.29}$$

which give(subtracting)

$$\psi^* \partial_\mu \partial^\mu \psi - \psi \partial_\mu \partial^\mu \psi^* = 0 \tag{20.30}$$

$$\partial_{\mu} \left(\psi^* \partial^{\mu} \psi - \psi \partial^{\mu} \psi^* \right) = 0 \tag{20.31}$$

Expanding these expressions, we have the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0 \tag{20.32}$$

where

$$\rho(\vec{r},t) = \frac{i\hbar}{2mc^2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right)$$
(20.33)

$$\vec{j}(\vec{r},t) = \frac{\hbar}{im} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right)$$
(20.34)

We have inserted a multiplicative constant so that the current density vector $\vec{j}(\vec{r},t)$ is identical to the nonrelativistic case. Because this density $\rho(\vec{r},t)$ satisfies a continuity equation, its integral over all space does not change in time. Clearly, however, it is not necessarily positive. In particular, $\rho < 0$ for a negative energy free particle eigenstate.

This means that we cannot interpret this new $\rho(\vec{r})$ as being the particle (probability) density at \vec{r} and we cannot interpret $\vec{j}(\vec{r})$ as a particle current.

The interpretation that will eventually emerge is that for charged particles $e\rho(\vec{r})$ represents the charge density at \vec{r} , which can have either sign and $e\vec{j}(\vec{r})$ represents the electric current at \vec{r} .

20.1.2 Negative Energy States and Antiparticles

How do we interpret the Klein-Gordon equation and its solutions?

Consider a free particle at rest, i.e., $\vec{p} = 0$. The wave function for the positive energy solution is

$$\psi(\vec{r},t) = e^{-imc^2 t/\hbar} \tag{20.35}$$

where the energy of a particle at rest is $E = mc^2$. The density for this state is $\rho(\vec{r}, t) = +1$.

Now make a Lorentz transformation to a new frame moving with velocity $-\vec{v}$ with respect to the particle at rest. The particle now appears to have a velocity \vec{v} in this new frame. It, therefore, has

momentum =
$$\vec{p} = \gamma m \vec{v}$$
 and energy = $E = \gamma m c^2$ (20.36)

where

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$
(20.37)

This result follows because

$$p_{\mu}x'^{\mu}$$
 = Lorentz scalar
= $-mc^2t$ in the rest frame
= $\vec{p} \cdot \vec{r}' - Et'$ in the moving frame

The new wave function

$$\psi(\vec{r}\,',t') = e^{i(\vec{p}\cdot\vec{r}\,'-Et')/\hbar} = e^{i(\vec{p}\cdot\vec{r}\,'-E_{\vec{p}}t')/\hbar} \tag{20.38}$$

is the result we expect for a particle of momentum \vec{p} and energy $E_{\vec{p}}$. If we calculate the density ρ for this wave function we get

$$\rho(\vec{r}\,',t') = \frac{E_{\vec{p}}}{mc^2} \tag{20.39}$$

and the current is

$$\vec{j}(\vec{r}\,',t') = \frac{\vec{p}}{m} = \frac{\vec{p}c^2}{E_{\vec{p}}}\rho(\vec{r}\,',t') = \vec{v}\rho(\vec{r}\,',t') \text{ (as expected)}$$
(20.40)

where

$$\vec{v} = \frac{\vec{p}c^2}{E_{\vec{p}}}$$
 (20.41)

We see that $\rho(\vec{r}, t)$ transforms like $E_{\vec{p}}$ or as the time component of a 4-vector, which makes physical sense. Since a unit volume in the rest frame appears smaller by a factor

$$1/\gamma = \sqrt{1 - v^2/c^2}$$
(20.42)

when observed from the moving frame, a unit density in the rest frame will appear as a density

$$\frac{1}{\gamma} = \frac{E_{\vec{p}}}{mc^2} \tag{20.43}$$

in a frame in which the particle is moving.

What about the negative energy solutions? For a particle at rest we have, in this case,

$$\psi(\vec{r},t) = e^{imc^2 t/\hbar} \tag{20.44}$$

where the energy of this particle at rest is $E = -mc^2$.

The density for this state is $\rho(\vec{r}, t) = -1$.

It turns out that one way to interpret a state with a negative particle density is to say that it is a state with a positive density of antiparticles.

We will make the interpretation that a particle at rest with energy $E = -mc^2$ is actually an antiparticle with positive energy $E = mc^2$. As we shall see,

this interpretation of negative energy states will lead to a consistent theoretical picture that is confirmed experimentally.

In a Lorentz frame traveling with velocity $-\vec{v}$ with respect to the antiparticle, the wave function is

$$\psi(\vec{r}\,',t') = e^{-i(\vec{p}\cdot\vec{r}\,'-Et')/\hbar} = e^{imc^2t/\hbar} \tag{20.45}$$

where

momentum
$$= \vec{p} = \gamma m \vec{v}$$
 and energy $= E = \gamma m c^2$ (20.46)

In this new frame the particle has velocity \vec{v} , momentum \vec{p} and energy $E_{\vec{p}}$. The wave function, however, describes a particle of energy $-E_{\vec{p}}$ and momentum $-\vec{p}$.

The density in the moving frame is

$$\rho(\vec{r}\,',t') = -\frac{E_{\vec{p}}}{mc^2} \tag{20.47}$$

and the current is

$$\vec{j}(\vec{r}\,',t') = -\frac{\vec{p}}{m}\rho(\vec{r}\,',t') = \frac{\vec{p}c^2}{E_{\vec{p}}}\rho(\vec{r}\,',t') \tag{20.48}$$

Thus, an antiparticle moving with velocity \vec{v} has associated with it a current moving in the opposite direction, i.e., a flow of antiparticles in one direction is equivalent to a flow of particles in the opposite direction.

For a charged particle $e\rho(\vec{r},t)$ is the charge density. It is positive for a free particle with e > 0 and negative for a free antiparticle, which has opposite charge to the particle.

The quantity $e\vec{j}(\vec{r},t)$ is the electric current of the state ψ . For a particle the electric current is in the direction of the particle velocity. For the antiparticle with e < 0, the electric current is opposite to the velocity.

This says that the interpretation of the negative energy solutions as antiparticles is consistent with the interpretation of the density ρ as a charge density and \vec{j} as an electric current.

Is this interpretation consistent with the way charged particles interact with the electromagnetic field?

The Klein-Gordon equation with an electromagnetic field present is given by

$$\frac{1}{c^2} \left(i\hbar \frac{\partial}{\partial t} - e\Phi(\vec{r}, t) \right)^2 \psi(\vec{r}, t) = \left(\left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}(\vec{r}, t) \right)^2 + m^2 c^2 \right) \psi(\vec{r}, t)$$
(20.49)

Taking the complex conjugate we have

$$\frac{1}{c^2} \left(i\hbar \frac{\partial}{\partial t} + e\Phi(\vec{r}, t) \right)^2 \psi^*(\vec{r}, t) = \left(\left(\frac{\hbar}{i} \nabla + \frac{e}{c} \vec{A}(\vec{r}, t) \right)^2 + m^2 c^2 \right) \psi^*(\vec{r}, t) \quad (20.50)$$

These equations say that if $\psi(\vec{r},t)$ is a solution to the Klein-Gordon equation with a certain sign of the charge, then $\psi^*(\vec{r},t)$ is a solution of the Klein-Gordon equation with the *opposite* sign of the charge and the *same* mass.

Thus, the relativistic theory of a spin zero particle predicts the existence of its antiparticle with the opposite charge and same mass, i.e., the theory contains solutions for both particles and antiparticles.

12pt] Relativistic invariance requires the existence of antiparticles

The complex conjugate of a negative energy solution is a positive energy solution with the opposite sign of the charge. The operation of taking the complex conjugate of the wave function will be called *charge conjugation*. Charge conjugation changes particles into antiparticles and vice versa. If we label quantities calculated with the complex conjugate wave function by a subscript \mathbf{c} , we find

$$\rho(\vec{r},t) = -\rho_c(\vec{r},t) \quad , \quad \vec{j}(\vec{r},t) = -\vec{j}_c(\vec{r},t) \tag{20.51}$$

as expected.

The solutions are normalized by the requirement that the total associated charge equals ± 1 unit, i.e.,

$$\int d^3 r \rho(\vec{r}, t) = +1 = -\int d^3 r \rho_c(\vec{r}, t)$$
(20.52)

This normalization is conserved in time and invariant under a Lorentz transformation.

20.2 Physics of the Klein-Gordon Equation

We first transform the Klein-Gordon equation into two equations, each first order in time.

We define

$$\psi^{0}(\vec{r},t) = \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)\psi(\vec{r},t) \qquad (1^{st} - \text{order equation }\#1) \qquad (20.53)$$

We then have

$$\left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)\psi^{0}(\vec{r},t) = \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)^{2}\psi(\vec{r},t)$$
(20.54)

Now using the Klein-Gordon equation we have

$$\left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)^2\psi(\vec{r},t) = c^2\left(\left(\nabla + \frac{ie}{\hbar c}\vec{A}(\vec{r},t)\right)^2 - \frac{m^2c^4}{\hbar^2}\right)\psi(\vec{r},t)$$
(20.55)

so we get

$$\left(\frac{\partial}{\partial t} + \frac{ie}{\hbar} \Phi(\vec{r}, t)\right) \psi^{0}(\vec{r}, t)$$

= $c^{2} \left(\left(\nabla + \frac{ie}{\hbar c} \vec{A}(\vec{r}, t) \right)^{2} - \frac{m^{2}c^{4}}{\hbar^{2}} \right) \psi(\vec{r}, t)$ (1st - order equation #2) (20.56)

These two new first-order equations involve the two functions $\psi^0(\vec{r},t)$ and $\psi(\vec{r},t)$.

Now define the linear combinations

$$\phi = \frac{1}{2} \left[\psi + \frac{i\hbar}{mc^2} \psi^0 \right] \quad , \quad \chi = \frac{1}{2} \left[\psi - \frac{i\hbar}{mc^2} \psi^0 \right] \tag{20.57}$$

Substitution then gives the more symmetric equations

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\phi = \frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2(\phi + \chi) + mc^2\phi \qquad (20.58)$$

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\chi = -\frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2(\phi + \chi) + mc^2\chi \qquad (20.59)$$

Now define a two-component wave function

$$\Psi(\vec{r},t) = \begin{pmatrix} \phi(\vec{r},t) \\ \chi(\vec{r},t) \end{pmatrix}$$
(20.60)

and three 2×2 matrices

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(20.61)

The two symmetric equations can then be combined into the single equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2(\tau_3 + i\tau_2) + mc^2\tau_3 + e\Phi\right]\Psi$$
(20.62)

This equation is completely equivalent to the original Klein-Gordon equation where

$$\psi = \phi + \chi \quad , \quad \psi^0 = \frac{mc^2}{i\hbar}(\phi - \chi) \tag{20.63}$$

The internal degree of freedom represented by these two components is the charge of the particle(one component represents the particle and the other the

antiparticle).

Using the two component equation, we can write the density as

$$\rho(\vec{r},t) = |\phi|^2 - |\chi|^2 = \Psi^+ \tau_3 \Psi$$
(20.64)

where $\Psi^+ = (\phi^*, \chi^*)$. A very simple expression. The current density, however, becomes less transparent

$$\vec{j}(\vec{r},t) = \frac{\hbar}{2im} \left[\Psi^{+} \tau_{3}(\tau_{3} + i\tau_{2}) \nabla \Psi - (\nabla \Psi^{+}) \tau_{3}(\tau_{3} + i\tau_{2}) \Psi \right] - \frac{e\vec{A}}{mc} \Psi^{+} \tau_{3}(\tau_{3} + i\tau_{2}) \Psi$$
(20.65)

The normalization condition becomes

$$\int d^3r \,\Psi^+ \tau_3 \Psi = \pm 1 \tag{20.66}$$

The scalar product between two such wave functions Ψ and |Psi'| is defined by

$$\langle \Psi \mid \Psi' \rangle = \int d^3 r \, \Psi^+(\vec{r}, t) \tau_3 \Psi'(\vec{r}, t) \tag{20.67}$$

Finally, the wave equation is of the form

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$$
 (20.68)

where the Hamiltonian is

$$\hat{H} = \left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2 (\tau_3 + i\tau_2) + mc^2\tau_3 + e\Phi \qquad (20.69)$$

Since $(\tau_3 + i\tau_2)^+ = \tau_3 - i\tau_2$, we find that $\hat{H}^+ \neq \hat{H}$, which seems to indicate that \hat{H} is not Hermitian. It is Hermitian, however, when we use the proper scalar product definition of hermiticity, i.e.,

$$\langle \Psi | \left(\hat{H} | \Psi' \right) \rangle = \left[\langle \Psi' | \left(\hat{H} | \Psi \right) \right]^*$$
(20.70)

This relation requires that

$$\tau_3 \hat{H}^+ \tau_3 = \hat{H}$$
 (20.71)

All required properties of Hermitian operators, i.e., real eigenvalues and so on, follow from the scalar product definition so that is all that is actually required.

Under the charge conjugation operation

$$\begin{cases} \phi \to \chi^* \\ \chi \to \phi^* \end{cases} \} \to \Psi_c = \tau_1 \Psi^*$$
 (20.72)

which is the form of the charge conjugation operation in two-component language.

We can now see the physical meaning of charge conjugation. Using

$$\vec{p}^* = \left(\frac{h}{i}\nabla\right)^* = -\frac{h}{i}\nabla = -\vec{p} \tag{20.73}$$

and $\tau_3 + i\tau_2$ = real matrix, we find that

$$\hat{H}^{*}(e) = \left[-\vec{p} - \frac{e}{c}\vec{A}\right]^{2} (\tau_{3} + i\tau_{2}) + mc^{2}\tau_{3} + e\Phi \qquad (20.74)$$

We then have

$$\tau_1 \hat{H}^*(e) \tau_1 = -\left[\vec{p} + \frac{e}{c}\vec{A}\right]^2 (\tau_3 + i\tau_2) - mc^2 \tau_3 + e\Phi = -\hat{H}(-e)$$
(20.75)

This means that, if Ψ solves the equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}(e)\Psi$$
 (20.76)

we have

$$-i\hbar\frac{\partial\Psi^*}{\partial t} = \hat{H}^*(e)\Psi^* = -\tau_1\hat{H}(-e)\tau_1\Psi^*$$
(20.77)

Multiplying by τ_1 we get

$$i\hbar\frac{\partial\Psi_c}{\partial t} = \hat{H}(-e)\Psi_c \tag{20.78}$$

which is the two-component statement of the fact that Ψ_c solves the Klein-Gordon equation with the opposite sign of the charge.

What can we say about the two-component solutions for free particles and antiparticles?

The wave function of a free particle (positive energy solution) of momentum \vec{p} (normalized to 1) is given by

$$\psi_{\vec{p}}^{(+)}(\vec{r},t) = \sqrt{\frac{mc^2}{E_{\vec{p}}}} e^{i(\vec{p}\cdot\vec{r}-E_{\vec{p}}t)/\hbar}$$
(20.79)

where

$$E_{\vec{p}} = \sqrt{p^2 c^2 + m^2 c^4} \tag{20.80}$$

Using

$$\psi^{0}(\vec{r},t) = \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)\psi(\vec{r},t)$$
(20.81)

and

$$\phi = \frac{1}{2} \left[\psi + \frac{i\hbar}{mc^2} \psi^0 \right] \quad , \quad \chi = \frac{1}{2} \left[\psi - \frac{i\hbar}{mc^2} \psi^0 \right] \tag{20.82}$$
we find (in two-component language)

$$\Psi_{\vec{p}}^{(+)}(\vec{r},t) = \Psi_{\vec{p}}^{(+)} e^{i(\vec{p}\cdot\vec{r}-E_{\vec{p}}t)/\hbar}$$
(20.83)

where the two-component vector $\Psi_{\vec{p}}^{(+)}$ is given by

$$\Psi_{\vec{p}}^{(+)} = \frac{1}{2\sqrt{E_{\vec{p}}mc^2}} \begin{pmatrix} mc^2 + E_{\vec{p}} \\ mc^2 - E_{\vec{p}} \end{pmatrix}$$
(20.84)

In a similar manner, we can write for the negative energy solutions (free antiparticles)

$$\psi_{\vec{p}}^{(-)}(\vec{r},t) = \sqrt{\frac{mc^2}{E_{\vec{p}}}} e^{-i(\vec{p}\cdot\vec{r}-E_{\vec{p}}t)/\hbar}$$
(20.85)

$$\Psi_{\vec{p}}^{(-)}(\vec{r},t) = \Psi_{\vec{p}}^{(-)} e^{-i(\vec{p}\cdot\vec{r}-E_{\vec{p}}t)/\hbar}$$
(20.86)

$$\Psi_{\vec{p}}^{(-)} = \frac{1}{2\sqrt{E_{\vec{p}}mc^2}} \begin{pmatrix} mc^2 - E_{\vec{p}} \\ mc^2 + E_{\vec{p}} \end{pmatrix} = \tau_1 \Psi_{\vec{p}}^{(+)}$$
(20.87)

We note that in the nonrelativistic limit

$$E_{\vec{p}} = \sqrt{p^2 c^2 + m^2 c^4} = mc^2 \left(1 + \frac{p^2}{m^2 c^2}\right)^{1/2} \approx mc^2 \left(1 + \frac{p^2}{2m^2 c^2}\right)$$
(20.88)

$$mc^2 \pm E_{\vec{p}} \approx \begin{cases} 2mc^2 \\ -p^2/2m \end{cases}$$
(20.89)

so that

$$\Psi_{\vec{p}}^{(+)} = \begin{pmatrix} 1 \\ -v^2/4c^2 \end{pmatrix} , \quad \Psi_{\vec{p}}^{(-)} = \begin{pmatrix} -v^2/4c^2 \\ 1 \end{pmatrix}$$
(20.90)

This shows that in the nonrelativistic limit

$$\chi \text{ is } \approx v^2/c^2 \text{ times } \phi \text{ for a particle}$$
 (20.91)

If we drop χ , then ϕ satisfies the nonrelativistic Schrodinger equation with the constant mc^2 included in the energy.

Similarly, dropping ϕ in the antiparticle solution shows that χ satisfies the nonrelativistic Schrodinger equation for the opposite charge with the constant mc^2 included in the energy.

The particle and antiparticle solutions are orthogonal in the sense that

$$\Psi_{\vec{p}}^{(+)}\tau_{3}\Psi_{\vec{p}}^{(-)} = 0 = \Psi_{\vec{p}}^{(-)}\tau_{3}\Psi_{\vec{p}}^{(+)}$$
(20.92)

which should be the case since they represent different energy eigenstates of the same Hamiltonian.

The free particle solutions form a complete set since any wave function Ψ can be expanded as a linear combination of the free particle and antiparticle solutions.

We first write Ψ as a Fourier transform

$$\Psi(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p}\cdot\vec{r}/\hbar} \begin{pmatrix} \phi_{\vec{p}} \\ \chi_{\vec{p}} \end{pmatrix}$$
(20.93)

Since the two vectors $\Psi_{\vec{p}}^{(+)}$ and $\Psi_{\vec{p}}^{(-)}$ are linearly independent, we can write

$$\Psi_{\vec{p}}(t) = \begin{pmatrix} \phi_{\vec{p}} \\ \chi_{\vec{p}} \end{pmatrix} = u_{\vec{p}}(t)\Psi_{\vec{p}}^{(+)} + v_{-\vec{p}}^*(t)\Psi_{-\vec{p}}^{(-)}$$
(20.94)

Good reasons for the choice of $-\vec{p}$ and * will appear shortly.

Substituting we get

$$\Psi(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p}\cdot\vec{r}/\hbar} \left[u_{\vec{p}}(t)\Psi_{\vec{p}}^{(+)} + v_{-\vec{p}}^*(t)\Psi_{-\vec{p}}^{(-)} \right]$$
$$= \int \frac{d^3p}{(2\pi\hbar)^3} \left[u_{\vec{p}}(t)\Psi_{\vec{p}}^{(+)}e^{i\vec{p}\cdot\vec{r}/\hbar} + v_{\vec{p}}^*(t)\Psi_{\vec{p}}^{(-)}e^{-i\vec{p}\cdot\vec{r}/\hbar} \right]$$
(20.95)

where a change of variables was made in the second term. From the form of this result, $u_{\vec{p}}(t)$ is the amplitude for a particle in the state Ψ to have momentum \vec{p} and positive charge and $v_{\vec{p}}(t)$ is the amplitude for a particle in the state Ψ to have momentum \vec{p} and negative charge.

Using the orthonormality of $\Psi_{\vec{p}}^{(\pm)}$ we get

$$u_{\vec{p}}(t) = \int d^3 r \Psi_{\vec{p}}^{(+)+} e^{-i\vec{p}\cdot\vec{r}/\hbar} \tau_3 \Psi(\vec{r},t)$$
(20.96)

$$v_{\vec{p}}^{*}(t) = -\int d^{3}r \Psi_{\vec{p}}^{(-)+} e^{i\vec{p}\cdot\vec{r}/\hbar} \tau_{3}\Psi(\vec{r},t)$$
(20.97)

The normalization integral for Ψ then becomes

$$\int \frac{d^3 p}{(2\pi\hbar)^3} \left(\left| u_{\vec{p}} \right|^2 - \left| v_{\vec{p}} \right|^2 \right) = \pm 1$$
(20.98)

This says that there is no restriction on the magnitude of either $u_{\vec{p}}$ or $v_{\vec{p}}$. Only the integral of the difference(above) is fixed.

Physically, we can then say that one can have a state with an arbitrarily large amplitude for finding a particle with a certain momentum, which is the first indication that we are dealing with *bosons* or that spin zero particles must be bosons.

We can write some expectation values in this formalism, i.e.,

$$\hat{H}_0 = \frac{p^2}{2m} (\tau_3 + i\tau_2)^2 + mc^2 \tau_3 = \text{Kineticenergy}$$
(20.99)

$$\int \Psi^{+}(\vec{r})\tau_{3}\hat{H}_{0}\Psi(\vec{r})d^{3}r = \int \frac{d^{3}p}{(2\pi\hbar)^{3}}E_{\vec{p}}\left(\left|u_{\vec{p}}\right|^{2} + \left|v_{\vec{p}}\right|^{2}\right)$$
(20.100)

and

$$\vec{p} = \frac{\hbar}{i} \nabla = \text{momentum}$$
 (20.101)

$$\int \Psi^{+}(\vec{r})\tau_{3}\left(\frac{\hbar}{i}\nabla\right)\Psi(\vec{r})d^{3}r = \int \frac{d^{3}p}{(2\pi\hbar)^{3}}\vec{p}\left(\left|u_{\vec{p}}\right|^{2} + \left|v_{\vec{p}}\right|^{2}\right)$$
(20.102)

20.3 Free Particles as Wave Packets

A wave packet formed from the positive energy solutions is given by

$$\Psi^{(+)}(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3} \, u_{\vec{p}} e^{i(\vec{p}\cdot\vec{r}-E_{\vec{p}}t)/\hbar} \Psi^{(+)}_{\vec{p}} \tag{20.103}$$

Let us assume that $u_{\vec{p}}$ is peaked about $\vec{p} = \vec{p}'$. Then, using arguments similar to our earlier discussions on stationary phase, the center of the wave packet moves with a group velocity

$$\vec{v}_g = \left(\nabla_{\vec{p}} E_{\vec{p}}\right)_{\vec{p}=\vec{p}\,'} = \frac{\vec{p}\,'c^2}{E_{\vec{p}\,'}} \tag{20.104}$$

and similarly for a free wave packet made of the negative energy solutions for antiparticles.

Can we construct a free particle wave packet perfectly localized at the origin? It would have the form

$$\Psi(\vec{r}) = \begin{pmatrix} a \\ b \end{pmatrix} \delta(\vec{r})$$
(20.105)

We then have

$$\begin{aligned} u_{\vec{p}} &= \int d^{3}r \Psi_{\vec{p}}^{(+)+} e^{-i\vec{p}\cdot\vec{r}/\hbar} \tau_{3} \Psi(\vec{r}) \\ &= \int d^{3}r \Psi_{\vec{p}}^{(+)+} e^{-i\vec{p}\cdot\vec{r}/\hbar} \tau_{3} \begin{pmatrix} a \\ b \end{pmatrix} \delta(\vec{r}) = \Psi_{\vec{p}}^{(+)+} \tau_{3} \begin{pmatrix} a \\ b \end{pmatrix} \\ &= \frac{1}{2\sqrt{E_{\vec{p}}mc^{2}}} \begin{pmatrix} mc^{2} + E_{\vec{p}} \\ mc^{2} - E_{\vec{p}} \end{pmatrix}^{+} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \\ &= \frac{E_{\vec{p}}(a+b) + mc^{2}(a-b)}{2\sqrt{E_{\vec{p}}mc^{2}}} \end{aligned}$$
(20.106)

and similarly

$$v_{\vec{p}}^* = -\Psi_{\vec{p}}^{(-)+} \tau_3 \begin{pmatrix} a \\ b \end{pmatrix} = \frac{E_{\vec{p}}(a+b) - mc^2(a-b)}{2\sqrt{E_{\vec{p}}mc^2}}$$
(20.107)

Looking at these results we can see that independent of the choice of a and b, the wave packet will always have both particle and antiparticle components. This means that it is impossible to construct a perfectly localized wave packet from positive energy solutions alone.

Suppose that we take a general wave packet made up of positive energy solutions and try to squeeze it(make it more localized) with real-world devices such as collimators. To see what might happen we multiply the wave packet by the position operator \vec{r} . We then have

$$\vec{r}\Psi^{(+)}(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3} u_{\vec{p}}(t)\Psi_{\vec{p}}^{(+)}\vec{r}e^{i\vec{p}\cdot\vec{r}/\hbar}$$
$$= \int \frac{d^3p}{(2\pi\hbar)^3} u_{\vec{p}}(t)\Psi_{\vec{p}}^{(+)}\frac{\hbar}{i}\nabla_{\vec{p}}e^{i\vec{p}\cdot\vec{r}/\hbar}$$
(20.108)

Integrating by parts we have

$$\vec{r}\Psi^{(+)}(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3} (i\hbar\nabla_{\vec{p}}u_{\vec{p}}(t))\Psi^{(+)}_{\vec{p}}e^{i\vec{p}\cdot\vec{r}/\hbar} + \int \frac{d^3p}{(2\pi\hbar)^3} u_{\vec{p}}(t)(i\hbar\nabla_{\vec{p}}\Psi^{(+)}_{\vec{p}})e^{i\vec{p}\cdot\vec{r}/\hbar}$$
(20.109)

Using

$$\nabla_{\vec{p}} \Psi_{\vec{p}}^{(\pm)} = -\frac{\vec{p}c^2}{2E_{\vec{p}}^2} \Psi_{\vec{p}}^{(\mp)}$$
(20.110)

we get

$$\vec{r}\Psi^{(+)}(\vec{r},t) = \vec{r}_{+}\Psi^{(+)}(\vec{r},t) + \vec{r}_{-}\Psi^{(+)}(\vec{r},t)$$
(20.111)

where

$$\vec{r}_{+}\Psi^{(+)}(\vec{r},t) = \int \frac{d^{3}p}{(2\pi\hbar)^{3}} (i\hbar\nabla_{\vec{p}}u_{\vec{p}}(t))\Psi^{(+)}_{\vec{p}}e^{i\vec{p}\cdot\vec{r}/\hbar}$$
(20.112)

$$\vec{r}_{-}\Psi^{(+)}(\vec{r},t) = -\int \frac{d^3p}{(2\pi\hbar)^3} u_{\vec{p}}(t) \frac{i\hbar\vec{p}c^2}{2E_{\vec{p}}^2} \Psi_{\vec{p}}^{(-)} e^{i\vec{p}\cdot\vec{r}/\hbar}$$
(20.113)

This says that multiplying a wave packet of positive energy states by the position operator mixes in negative energy solutions, i.e.,

 \vec{r}_{+} generates positive energy solutions while \vec{r}_{-} generates negative energy solutions

or changes free particles in free antiparticles and vices versa

The same result occurs for any function of the position operator.

Suppose that $\vec{r}\Psi^{(+)}(\vec{r}) = \vec{r}_0\Psi^{(+)}(\vec{r})$, i.e., it is an eigenstate of \vec{r} with eigenvalue \vec{r}_0 . This says that

$$i\hbar \nabla_{\vec{p}} u_{\vec{p}} = \vec{r}_0 u_{\vec{p}} \to u_{\vec{p}} = e^{-i\vec{p}\cdot\vec{r}_0/\hbar}$$
 (20.114)

and the state

$$\Psi_{\vec{r}_0}^+(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p}\cdot(\vec{r}-\vec{r}_0)/\hbar} \Psi_{\vec{p}}^{(+)}$$
(20.115)

is an eigenstate of \vec{r}_+ .

This eigenstate is not normalizable. It is large over a region of space within \hbar/mc (a Compton wavelength) of \vec{r}_0 or, in other words, the theory with positive energy solutions cannot describe particles localized to a region smaller than a Compton wavelength.

The presence of the \vec{r}_{-} part in the position operator says that putting a wave packet made from positive energy solutions (a particle) through a potential $\Phi(\vec{r})$ (which multiplies by functions of r) causes the creation of antiparticles and because charge must be conserved, creates new particles also.

Thus, the relativistic spin-zero theory of the Klein-Gordon equation has built into it the mechanism of particle-antiparticle production by external potentials.

An example of this phenomenon is *Klein's paradox*. Suppose we have a beam of positively charged particles with momentum p hitting an electrostatic potential barrier of height $e\varphi$ from the left as shown in Figure 20.1 below.



Figure 20.1: Electrostatic Potential Barrier - Klein Paradox

The solution follows the same lines as the nonrelativistic problem. For x < 0 we have

 $\psi(x) = ae^{ipx/\hbar} + be^{-ipx/\hbar}$, Energy = E_p (20.116)

This corresponds to incident and reflected waves. For x > 0, the Klein-Gordon equation is

$$(E_p - V)^2 \psi(x) = -\hbar^2 c^2 \frac{\partial^2 \psi(x)}{\partial x^2} + mc^2 \psi(x) \quad , \quad V = e\varphi \tag{20.117}$$

The solution takes the form $\psi(x) = de^{ikx}$ where substitution gives

$$(E_p - V)^2 = \hbar^2 c^2 k^2 + m^2 c^4$$
(20.118)

We have the boundary conditions at x = 0 (since potential only has a finite discontinuity)

$$\psi(x), \frac{\partial \psi}{\partial x} \text{ continuous}$$
(20.119)

Note that ψ^0 is given by

$$\psi^{0}(\vec{r},t) = \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)\psi(\vec{r},t)$$
(20.120)

is not continuous at x = 0.

We obtain

$$b = \frac{p - \hbar k}{p + \hbar k} a \quad , \quad d = \frac{2p}{p + \hbar k} a \tag{20.121}$$

We consider three cases:

- 1. If $E_p > V + mc^2$, then the particle can pass the over the barrier and the results are identical to the nonrelativistic case, i.e., part of the wave is reflected and part is transmitted.
- 2. If we have a stronger potential such that $E_p + mc^2 > V > E_p mc^2$, then k must be imaginary so that the wave function goes to zero as $x \to \infty$. We then have

$$k = i\kappa \to \kappa = \frac{\sqrt{m^2 c^4 - (E_p - V)^2}}{\hbar c}$$
(20.122)

and the wave is totally reflected at the barrier. The charge density on the right (x > 0) is given by

$$\rho(x) = \frac{E_p - V}{2mc^2} \left| d \right|^2 e^{-2\kappa x}$$
(20.123)

For $E_p > V$, there exists a positive, exponentially decaying charge density to the right of the barrier. For $E_p < V$, however, the density is *negative* (remember it is a beam of positive particles). We reflect positively charged particles from the barrier and find negative particles inside the barrier.

3. We make the potential even stronger so that $V > E_p + mc^2$. Nonrelativistically it would be even more impossible for the particles to pass over the barrier. In the relativistic case, however, k is real again, This says that once again there is a particle current to the right of the barrier. The group velocity of the waves for x > 0 is

$$v_g = \frac{\partial E_p}{\partial(\hbar k)} \tag{20.124}$$

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Using $(E_p - V)^2 = \hbar^2 c^2 k^2 + m^2 c^4$ we get

$$(E_p - V)\frac{\partial E_p}{\partial k} = \hbar c^2 k \to v_g = \frac{\hbar c^2 k}{E_p - V}$$
(20.125)

Since $E_p - V < 0$, we must have k < 0 (negative!) in order to have a wave(packet) traveling from the barrier towards positive x.

This says that the reflection coefficient b/a is greater than one, i.e., more wave is reflected than is incident! In addition, the charge density on the right is

$$\rho(x) = \frac{E_p - V}{2mc^2} \left| d \right|^2 < 0 \tag{20.126}$$

and the current on the right is negative.

One possible explanation is to say that the incident particle induces the creation of particle-antiparticle pairs at the barrier. The created antiparticles, having the opposite charge, find x > 0 a region of attractive potential and thus travel towards the right, which explains the negative current on the right. The created particles travel to the left and together with the incident particles (wave) which are(is) totally reflected, they add up to an outgoing current on the left that is larger than the incident current.

The total outgoing current on the left and right equals the incident current since total charge must be conserved.

This pair creation solution does not violate conservation of energy. The energy of a created particle on the left is E_p . The energy of a created antiparticle on the right is $\sqrt{\hbar^2 c^2 k^2 + m^2 c^4} - V$ since the electrostatic potential energy has the opposite sign for a particle of opposite charge.

Adding the two energies we get $E_p + \sqrt{\hbar^2 c^2 k^2 + m^2 c^4} - V = 0$, i.e., it takes zero energy to create a particle-antiparticle pair. This happens because the potential V is so large that the energy of the antiparticle on the right is not only less than mc^2 but is negative.

20.4 Bound State Problems

We now study the bound states of spin zero relativistic particles in a static potential $\Phi(\vec{r})$. For a positively charged particle with energy E the bound state wave function is

$$\psi(\vec{r},t) = e^{-iEt/\hbar}\psi(\vec{r})$$
 (20.127)

and the charge density of the bound state particle is

$$e\rho(\vec{r}) = \frac{e[E - e\Phi(\vec{r})]}{mc^2} |\psi(\vec{r})|^2$$
(20.128)

This says that in regions where $E > e\Phi(\vec{r})$, which includes classically accessible regions, the charge density is positive. But, in regions where $E < e\Phi(\vec{r})$, the charge density is negative. The way to think about this is to say the particle in the potential is a linear combination of free particle and free antiparticle states.

Because we are considering an electrostatic potential, the positively charged parts will be found mainly in regions of smaller $e\Phi(\vec{r})$ while the negatively charged parts will be found in regions of larger $e\Phi(\vec{r})$. A relativistic particle seems to have an internal structure that can be polarized by and electric field.

Alternatively, we might say that the potential produces particle-antiparticle pairs in the vacuum, The positively charged particles are attracted to regions of smaller $e\Phi(\vec{r})$ while the negatively charged particles are attracted to regions of larger $e\Phi(\vec{r})$. We say that the electric potential has *polarized* the vacuum. This polarization modifies the effective potential felt by the bound particle.

This interaction cannot be taken into account in the present one-particle relativistic theory(requires quantum field theory).

We now turn to the problem of a spin zero particle bound in a Coulomb potential. An example is a π^- bound to a nucleus. We have

$$e\Phi(\vec{r}) = -\frac{Ze^2}{r} \tag{20.129}$$

which leads to the Klein-Gordon equation

$$\left[\left(E + \frac{Ze^2}{r} \right)^2 + \hbar^2 c^2 \nabla^2 - mc^2 \right] \psi(\vec{r}) = 0$$
 (20.130)

Since this is a central potential, we can assume that the eigenstates have definite values of total orbital angular momentum. We then have

$$\left[\left(\frac{E^2}{c^2} - m^2 c^2 \right) + \hbar^2 \left(\frac{1}{r} \frac{\partial^2}{\partial r^2} r - \frac{\ell(\ell+1) - (Z\alpha)^2}{r^2} \right) + \frac{2Ze^2}{r} \frac{E}{c} \right] \psi(r) = 0 \quad (20.131)$$

or

$$\left[-\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\ell(\ell+1) - (Z\alpha)^2}{r^2} - \frac{2Z\alpha E}{\hbar cr} - \left(\frac{E^2 - m^2 c^4}{\hbar^2 c^2}\right)\right]\psi(r) = 0 \qquad (20.132)$$

where

$$\alpha = \frac{e^2}{\hbar c} = \text{ fine structure constant}$$
(20.133)

Now we define

$$\begin{split} \gamma &= Z\alpha \quad , \quad \ell'(\ell'+1) = \ell(\ell+1) - \gamma^2 \\ \lambda &= \frac{2E\gamma}{\hbar c\sigma} \quad , \quad \frac{4(m^2c^4 - E^2)}{\hbar^2c^2} = \sigma^2 \quad , \quad \rho = \sigma r \end{split}$$

and we get

$$\left[\frac{d^2}{d(\rho/2)^2} + \frac{2\lambda}{\rho/2} - 1 + \frac{\ell'(\ell'+1)}{(\rho/2)^2}\right]\rho\psi(\rho) = 0$$
(20.134)

which is identical to the radial equation for the nonrelativistic Coulomb problem for the function $u = \rho\psi(\rho)$. The difference is that ℓ' is not necessarily an integer (remember that it is an integer in the nonrelativistic problem), which causes the orbits of the relativistic Coulomb (Kepler) problem to no longer be closed, i.e., the orbits precess. This also means that the extra degeneracy of the nonrelativistic problem which causes the energy to be independent of ℓ is broken in the relativistic problem. We now solve this equation in the standard way. For

$$\rho \to 0 \qquad \psi(\rho) \to \rho^{\ell'}$$
$$\rho \to \infty \qquad \psi(\rho) \to e^{-\rho/2}$$

Therefore, we guess a solution of the form

$$u = \rho \psi(\rho) = \left(\frac{\rho}{2}\right)^{\ell'+1} e^{-\rho/2} w(\rho/2)$$
(20.135)

The solution method is identical to the nonrelativistic hydrogen atom. We get a power series which must terminate (so that the solution is normalizable) when

$$\lambda = N + \ell' + 1 \quad , \quad N = 0, 1, 2, 3, \dots$$

$$E = mc^2 \left(1 + \frac{\gamma^2}{\lambda^2}\right)^{-1/2} \rightarrow E = \frac{mc^2}{\sqrt{1 + \frac{\gamma^2}{\left[N + \frac{1}{2} + \sqrt{(\ell + \frac{1}{2})^2 - \gamma^2}\right]^2}}$$
(20.136)

If we define the principal quantum number $n = N + \ell + 1$ = integer, then we have

$$E_{n\ell} = \frac{mc^2}{\sqrt{1 + \frac{\gamma^2}{\left[n - (\ell + \frac{1}{2}) + \sqrt{(\ell + \frac{1}{2})^2 - \gamma^2}\right]^2}}}$$
(20.137)

The principal quantum number has the possible values $n = 1, 2, 3, \dots$ For a given *n* the possible values of the total orbital angular momentum are $\ell = 0, 1, 2, 3, \dots, n-1$.

The degeneracy that was present in the nonrelativistic theory with respect to orbital angular momentum ℓ is clearly removed.

If we expand the energy in a power series in the fine structure constant α (or γ) we get

$$E_{n\ell} = mc^2 - Ry\frac{1}{n^2} - Ry\frac{\gamma^2}{n^3} \left(\frac{1}{\ell + \frac{1}{2}} - \frac{3}{4n}\right) + O(Ry\gamma^4)$$
(20.138)

The first term is the rest energy. The second term is the nonrelativistic Rydberg formula. The third term is the relativistic correction due to using the relativistic form of the kinetic energy, which as we saw earlier in Chapter 10 took the form

$$\hat{H}_{rel} = -\frac{p^4}{8m^3c^2} \tag{20.139}$$

It is this correction that removes the degeneracy in ℓ , i.e.,

$$E_{n,\ell=0} - E_{n,\ell=n-1} = Ry \frac{4\gamma^2}{n^3} \frac{n-1}{2n-1}$$
(20.140)

As we shall see later when we derive the Dirac equation, there are more corrections to this formula due to the fact that the electron has spin = 1/2.

20.4.1 Nonrelativistic Limit

The Klein-Gordon equation in the presence of an electromagnetic field is

$$\frac{1}{c^2} \left(i\hbar \frac{\partial}{\partial t} - e\Phi(\vec{r}, t) \right)^2 \psi(\vec{r}, t) = \left(\left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}(\vec{r}, t) \right)^2 + m^2 c^2 \right) \psi(\vec{r}, t) \quad (20.141)$$

and using

$$\psi(\vec{r},t) = \begin{pmatrix} \phi(\vec{r},t) \\ \chi(\vec{r},t) \end{pmatrix}$$
(20.142)

we have as earlier

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\phi = \frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2\phi + mc^2\phi + \frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2\chi \qquad (20.143)$$

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\chi = -\frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2(\phi + \chi) - mc^2\chi$$
(20.144)

Remember that in the nonrelativistic limit the dominant term in the energy will be mc^2 so that we expect the zeroth order equation for χ to be

$$i\hbar\frac{\partial\chi}{\partial t} = mc^2\chi \tag{20.145}$$

which then implies in the next approximation that

$$\chi = -\frac{1}{4m^2c^2} \left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2 \phi \qquad (20.146)$$

and that ϕ satisfies the equation

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\phi = \frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2\phi + mc^2\phi - \frac{1}{8m^3c^2}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^4\phi \quad (20.147)$$

The operator on the right-hand side is just the kinetic energy operator

$$\sqrt{m^2 c^4 + c^2 \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}\right)^2} \tag{20.148}$$

expanded to second order in $1/mc^2$. This agrees with our earlier result that the first relativistic correction for a spinless particle is entirely due to the relativistic modification of the kinetic energy.

For a weak magnetic field \vec{B} this becomes (to order $(v/c)^3$) after much algebra

$$i\hbar\frac{\partial\phi}{\partial t} = -\frac{\hbar^2\nabla^2}{2m} \left[1 + \frac{\hbar^2\nabla^2}{2m^2c^2}\right]\phi + (mc^2 + e\Phi)\phi - \frac{e}{2mc}\vec{B}\cdot\vec{L}\left[1 + \frac{\hbar^2\nabla^2}{2m^2c^2}\right]\phi \quad (20.149)$$

where \vec{L} is the orbital angular momentum of the particle. The term

$$\left[1 + \frac{\hbar^2 \nabla^2}{2m^2 c^2}\right] \rightarrow \left[1 - \frac{p^2}{2m^2 c^2}\right] \tag{20.150}$$

represents the relativistic correction to the magnetic moment.

20.5 Relativistic Spin 1/2 Particles - The Dirac Equation

20.5.1 Lorentz Transformation of Spin

The contravariant and covariant components of the position 4-vector in spacetime are:

$$\begin{array}{lll} x^{\mu}: & x^{0}=ct & , & x^{1}=x & , & x^{2}=y & , & x^{3}=z \\ x_{\mu}: & x^{0}=ct & , & x_{1}=-x & , & x_{2}=-y & , & x_{3}=-z \end{array}$$

The flat spacetime metric tensor is defined by

$$g = (g_{\mu\nu}) = (g^{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$
(20.151)

The metric tensor relates covariant and contravariant components by

$$x_{\mu} = g_{\mu\nu} x^{\nu} \quad , \quad x^{\mu} = g^{\mu\nu} x_{\nu} \tag{20.152}$$

We also have

$$g^{\mu}_{\nu} = g^{\mu\alpha}g_{\alpha\nu} \equiv \delta^{\mu}_{\nu} \quad , \quad (\delta^{\mu}_{\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
(20.153)

Under the action of a Lorentz transformation along the z-axis with velocity $v = \beta c$, a 4-vector (any type) since it is a first-rank tensor, transforms as

$$V^{\prime\mu} = \Lambda^{\mu}_{\nu} V^{\nu} \tag{20.154}$$

where

$$(\Lambda^{\mu}_{\nu}) = \begin{pmatrix} \gamma & 0 & 0 & -\beta\gamma \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\beta\gamma & 0 & 0 & \gamma \end{pmatrix} \quad , \quad \gamma = \frac{1}{\sqrt{1-\beta^2}} \quad , \quad \beta = \frac{v}{c}$$
(20.155)

This corresponds to the standard transformation relations for the position and momentum 4-vectors

$$ct' = \gamma(ct - \beta z) , \quad x' = x , \quad y' = y , \quad z' = \gamma(z - \beta ct)$$
$$\frac{E'}{c} = \gamma\left(\frac{E}{c} - \beta p_z\right) , \quad p'_x = p_x , \quad p'_y = p_y , \quad p'_z = \gamma\left(p_z - \beta \frac{E}{c}\right)$$

Spin is an angular momentum corresponding to internal degrees of freedom of the system. This means, as we showed earlier, that spin must have the same transformation properties as any other angular momentum.

Nonrelativistically, we think of angular momentum as a vector and, in fact, under a simple spatial rotation it does transform as a vector (as we saw earlier). Consider, however, the behavior of an orbital angular momentum

$$\vec{L} = \vec{r} \times \vec{p} \to L_i = \varepsilon_{ijk} x_j p_k \tag{20.156}$$

under the action of a Lorentz transformation along the $z{\rm -direction}.$ We find that

$$L'_{z} = x'p'_{y} - y'p'_{x} = xp_{y} - yp_{x} = L_{z}$$
(20.157)

since the components of vectors orthogonal to the z-axis are unchanged. This is clearly not the transformation property of a vector.

In fact, \vec{L} is the product of two vectors and therefore should have the transformation properties of a second-rank tensor, i.e., as

$$Q'^{\mu\nu} = \Lambda^{\mu}_{\alpha} \Lambda^{\nu}_{\beta} Q^{\alpha\beta} \tag{20.158}$$

Relativistic electrodynamics can be written in terms of a second-rank field tensor

$$(F^{\mu\nu}) = \begin{pmatrix} 0 & \varepsilon_1 & \varepsilon_2 & \varepsilon_3 \\ -\varepsilon_1 & 0 & B_3 & -B_2 \\ -\varepsilon_2 & -B_3 & 0 & B_1 \\ -\varepsilon_3 & B_2 & -B_1 & 0 \end{pmatrix}$$
(20.159)

as Maxwell's equations

$$\begin{aligned} \frac{\partial F^{\mu\nu}}{\partial x^{\mu}} &= \frac{4\pi}{c} J^{\nu} \\ \frac{\partial F^{\mu\nu}}{\partial x^{\alpha}} + \frac{\partial F^{\nu\alpha}}{\partial x^{\mu}} + \frac{\partial F^{\alpha\mu}}{\partial x^{\nu}} = 0 \end{aligned}$$

where the current density 4-vector is

$$J^{\mu} = (c\rho, J_x, J_y, J_z)$$
(20.160)

and the Lorentz force law is

$$\frac{dp^{\mu}}{d\tau} = \frac{q}{m} p_{\nu} F^{\mu\nu} \tag{20.161}$$

The transformation rule then says that the fields transform according to the relations

$$F'^{01} = \varepsilon'_1 = \Lambda^{\mu}_{\alpha} \Lambda^{\nu}_{\beta} F^{\alpha\beta} = \Lambda^0_{\alpha} \Lambda^1_{\beta} F^{\alpha\beta} = \Lambda^0_{\alpha} \Lambda^1_1 F^{\alpha 1} = \Lambda^0_{\alpha} F^{\alpha 1}$$
$$= \Lambda^0_0 F^{01} + \Lambda^0_3 F^{31} = \gamma \varepsilon_1 - \beta \gamma B_2 = \gamma (\varepsilon_1 - ((\vec{v}/c) \times \vec{B})_1)$$

or

$$\varepsilon_1' = \gamma(\varepsilon_1 + ((\vec{v}/c) \times \vec{B})_1) \text{ where } \vec{v} = v\hat{e}_z$$
(20.162)

Similarly, we find

$$\begin{aligned} \varepsilon_2' &= \gamma(\varepsilon_2 + ((\vec{v}/c) \times \vec{B})_2) \quad , \quad \varepsilon_3' = \varepsilon_3 \\ B_1' &= \gamma(B_1 - ((\vec{v}/c) \times \vec{\varepsilon})_1) \quad , \quad B_2' = \gamma(B_2 - ((\vec{v}/c) \times \vec{\varepsilon})_2) \quad , \quad B_3' = B_3 \end{aligned}$$

We can summarize these results for an arbitrary (direction) Lorentz transformation applied to a second-rank tensor by

$$\begin{split} B'_{\parallel} &= B_{\parallel} \quad , \quad \varepsilon'_{\parallel} = \varepsilon_{\parallel} \parallel = \text{ component parallel to } \vec{v} \\ \vec{B}'_{\perp} &= \gamma \left(\vec{B}_{\perp} - (\vec{v}/c) \times \vec{\varepsilon} \right) \\ \vec{\varepsilon}'_{\perp} &= \gamma \left(\vec{\varepsilon}_{\perp} + (\vec{v}/c) \times \vec{B} \right) \perp = \text{ component perpendicular to } \vec{v} \end{split}$$

Thus, a pure magnetic field in one frame is a mixture of magnetic and electric fields in the new frame.

Now, under a spatial inversion transformation, we have

$$\begin{split} \vec{\varepsilon} &\to -\vec{\varepsilon} \quad , \quad \vec{B} \to \vec{B} \\ \vec{r} &\to -\vec{r} \quad , \quad \vec{p} \to -\vec{p} \Rightarrow \vec{L} \to \vec{L} \end{split}$$

Therefore, an angular momentum (including spin) has the same transformation properties as the magnetic field.

Since spin,

$$\bar{S} = \frac{1}{2}\vec{\sigma} \tag{20.163}$$

must transform as an angular momentum, which transforms like a magnetic field and the magnetic field is part of second-rank tensor with the electric field, we must conclude that there exists another set of dynamical variables generated

by the internal degrees of freedom of the particle that will be analogous to the electric field. Do not think of the operator $\vec{\sigma}$ as the standard 2×2 Pauli matrices; we shall see later that $\vec{\sigma}$ will need to be represented by 4×4 matrices relativistically.

We define these new variables as $i\vec{\alpha}/2$ where the i/2 factor is chosen for later convenience. We then have that \vec{S} and $i\vec{\alpha}/2$ or $\vec{\sigma}$ and $i\vec{\alpha}$ transform as \vec{B} and $\vec{\varepsilon}$, i.e.,

$$\begin{split} \sigma'_{\parallel} &= \sigma_{\parallel} \quad , \quad \vec{\sigma}'_{\perp} &= \gamma \left(\vec{\sigma}_{\perp} - (\vec{v}/c) \times i \vec{\alpha} \right) \\ i\alpha'_{\parallel} &= i\alpha_{\parallel} \quad , \quad i\vec{\alpha}'_{\perp} &= \gamma \left(i\vec{\alpha}_{\perp} + (\vec{v}/c) \times \vec{\sigma} \right) \end{split}$$

and they form a second-rank tensor $\sigma^{\mu\nu}$ analogous to $F^{\mu\nu}$, i.e.,

$$(\sigma^{\mu\nu}) = \begin{pmatrix} 0 & i\alpha_1 & i\alpha_2 & i\alpha_3 \\ -i\alpha_1 & 0 & \sigma_3 & -\sigma_2 \\ -i\alpha_2 & -\sigma_3 & 0 & \sigma_1 \\ -i\alpha_3 & \sigma_2 & -\sigma_1 & 0 \end{pmatrix}$$
(20.164)

We must now investigate the dynamical properties of the new variables $\vec{\alpha}$ and also ask this question - where have these objects been hiding in all of previous discussions?

Since spin is an angular momentum, we know its algebraic properties (commutators). In addition, spin generates rotations of the internal degrees of freedom. Spin commutes with spatial degrees of freedom like \vec{r} and \vec{p} and, thus, so does $\vec{\alpha}$.

Since $\vec{\alpha}$ behaves like a vector under spatial rotations (it is like the electric field vector), it must have the standard commutation relations with \vec{S}

$$[\alpha_i, S_j] = i\varepsilon_{ijk}\alpha_k \to [\alpha_i, \sigma_j] = 2i\varepsilon_{ijk}\alpha_k \tag{20.165}$$

Since $\vec{\sigma}$ is angular momentum, it satisfies the relations

$$\sigma_i \sigma_j = i \varepsilon_{ijk} \sigma_k + \delta_{ij} \tag{20.166}$$

which must be true in all Lorentz frames, i.e., since $\sigma_1^2 = 1$, we must have $\sigma_1'^2 = 1$.

Let us now determine all the properties of $\vec{\alpha}$.

For a Lorentz transformation along the z-direction we have

$$\sigma'_{x} = \gamma \left(\sigma_{x} + iv\alpha_{y}/c \right)$$

$$\sigma'_{y} = \gamma \left(\sigma_{y} - iv\alpha_{x}/c \right)$$

Squaring σ'_x we get

$$\sigma_x^{\prime 2} = 1 = \gamma^2 \left(\sigma_x^2 + iv(\sigma_x \alpha_y + \alpha_y \sigma_x)/c - (v/c)^2 \right) \alpha_y^2 \right)$$
$$= \gamma^2 \left(1 - (v/c)^2 \right) \alpha_y^2 \right) + \gamma^2 \left(iv(\sigma_x \alpha_y + \alpha_y \sigma_x)/c \right)$$

Since this must be true for all v, the coefficient of v/c must vanish. Thus,

$$\sigma_x \alpha_y + \alpha_y \sigma_x = 0 \tag{20.167}$$

We then have

$$1 = \gamma^2 \left(1 - (v/c)^2 \right) \alpha_y^2 \right)$$
(20.168)

Since

$$1 = \gamma^2 \left(1 - (v/c)^2 \right) \alpha_y^2 \right)$$
(20.169)

we must also have

$$\alpha_y^2 = 1 \tag{20.170}$$

These results generalize to the following:

$$i \neq j$$
 $\sigma_i \alpha_j = -\alpha_j \sigma_i$ (20.171)

$$i = j \qquad [\sigma_i, \alpha_i] = 0 \tag{20.172}$$

Multiplying σ'_y by σ'_x we get

$$\sigma'_x \sigma'_y = i\sigma'_z = i\sigma_z = \gamma^2 \left(\sigma_x + iv\alpha_y/c\right) \left(\sigma_y - iv\alpha_x/c\right)$$
$$i\sigma_z = \gamma^2 \left(\sigma_x \sigma_y + (v/c)^2 \alpha_y \alpha_x + i(v/c)(\alpha_y \sigma_y - \sigma_x \alpha_x)\right)$$

Multiplying σ'_x by σ'_y we get

$$\sigma'_{y}\sigma'_{x} = -i\sigma'_{z} = -i\sigma_{z} = \gamma^{2} \left(\sigma_{y} - iv\alpha_{x}/c\right) \left(\sigma_{x} + iv\alpha_{y}/c\right)$$
$$-i\sigma_{z} = \gamma^{2} \left(\sigma_{y}\sigma_{x} + (v/c)^{2}\alpha_{x}\alpha_{y} + i(v/c)(\sigma_{y}\alpha_{y} - \alpha_{x}\sigma_{x}\right)$$

Adding, we have

$$(\sigma_y \sigma_x + \sigma_x \sigma_y) + (v/c)^2 (\alpha_x \alpha_y + \alpha_y \alpha_x) = 0$$
$$(\alpha_x \alpha_y + \alpha_y \alpha_x) = 0 \rightarrow (\alpha_i \alpha_j + \alpha_j \alpha_i) = 0 \quad i \neq j$$

Continuing, we find these other relations

$$\alpha_y \alpha_x = -i\sigma_z = -\alpha_x \alpha_y \to \alpha_i \alpha_j - \alpha_j \alpha_i = 2i\varepsilon_{ijk}\sigma_k \tag{20.173}$$

or summarizing we have

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \quad , \quad [\alpha_i, \alpha_j] = 2i\varepsilon_{ijk}\sigma_k \tag{20.174}$$

$$[\alpha_i, \sigma_j] = 2i\varepsilon_{ijk}\alpha_k \quad , \quad \{\alpha_i, \sigma_j\} = 0 \quad , \quad i \neq j$$
(20.175)

So α obeys exactly the same algebraic relations as σ . How do we know that α is not equal to σ ? If we apply a parity transformation, we find that $\vec{\sigma} \rightarrow \vec{\sigma}$ since angular momentum is unchanged by spatial inversion, i.e., the space-space components of a second-rank tensor do not change sign under parity. On the other hand, the time-space components such as the electric field or $i\vec{\alpha}$ do change sign, i.e., $\vec{\alpha} \rightarrow -\vec{\alpha}$. So they cannot be the same operator!

Let β be the operator that corresponds to the parity transformation in spin space. Now two successive inversions brings us back to the starting configuration. Remember, however, that the spin representation of rotations is doubled valued, i.e., a rotation by 2π produces a minus sign. We have a choice of letting the square of the parity operation include a 2π rotation(about any axis) or not. This means that we can have $\beta^2 = +1$ or -1.

In the first case, the eigenvalues of β are ± 1 and in the second case $\pm i$. We choose $\beta^2 = +1 \rightarrow \beta^{-1} = \beta$. The properties under parity become

$$\beta^{-1}\vec{\sigma}\beta = \vec{\sigma} \to \beta\vec{\sigma} = \vec{\sigma}\beta \tag{20.176}$$

$$\beta^{-1}\vec{\alpha}\beta = -\vec{\alpha} \to \beta\vec{\alpha} = -\vec{\alpha}\beta \tag{20.177}$$

We can now construct an explicit matrix representation for the operators $\vec{\alpha}$, β and $\vec{\sigma}$ similar to the two-dimensional Pauli matrix representation in the nonrelativistic case.

Consider the determinant of the matrix for $\beta^{-1}\alpha_i\beta$. Using $\beta\vec{\alpha} = -\vec{\alpha}\beta$ we have

$$\det(\beta^{-1}\alpha_i\beta) = \det(-\beta^{-1}\beta\alpha_i) = \det(-\alpha_i) = (-1)^N \det(\alpha_i)$$
(20.178)

where N is the dimension of the matrix representation. However, using the cyclic property of determinants, i.e.,

$$\det ABC = \det BCA = \det CAB \tag{20.179}$$

we get

$$\det(\beta^{-1}\alpha_i\beta) = \det(\beta\beta^{-1}\alpha_i) = \det(\alpha_i)$$
(20.180)

Putting these results together we get

$$(-1)^N \det(\alpha_i) = \det(\alpha_i) \to (-1)^N = 1 \to N = 2, 4, 6, \dots$$
 (20.181)

We have used the fact that $det(\alpha_i) \neq 0$, since $\alpha_i^2 = 1$.

Now, N = 2 is not possible as we show below.

All 2×2 matrices can be constructed from the set $\{I, \vec{\sigma}\}$ and $[\beta, \vec{\sigma}] = 0$. This means that β would have to commute with all 2×2 matrices. Since $\vec{\alpha}$ would then have to commute with β , we would then violate the relation $\beta \vec{\alpha} = -\vec{\alpha}\beta$.

This means N must be at least as large as 4. This says that a relativistic spin 1/2 particle would have 4 internal states (the nonrelativistic case has 2). This is similar to the Klein-Gordon case and it will turn out here also that this doubling signals the appearance of antiparticles.

An explicit representation (not unique) using the 2×2 matrices

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \quad \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where the last three matrices are the standard Pauli matrices. It is given by

$$\vec{\sigma} = \begin{pmatrix} \vec{\tau} & 0\\ 0 & \vec{\tau} \end{pmatrix} \quad , \quad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\tau}\\ \vec{\tau} & 0 \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} I & 0\\ 0 & -I \end{pmatrix}$$
(20.182)

Note that the trace of each of these matrices is zero, which is a general property of matrices that obey anticommutation relations.

We can make the following physical interpretations of the components of the tensor $\sigma^{\mu\nu}.$

It follows from earlier discussions that the space-space components, i.e., the spin operators σ_j , generate (in the spin degrees of freedom) a rotation of the coordinate system.

This implies that the operators $\vec{\sigma}', \vec{\alpha}', \beta'$ in a spatially rotated frame are given by the operator relations

$$\vec{\sigma}' = R_{\varphi}\vec{\sigma}R_{\varphi}^{-1}, \quad \vec{\alpha}' = R_{\varphi}\vec{\alpha}R_{\varphi}^{-1}, \quad \beta' = R_{\varphi}\beta R_{\varphi}^{-1}$$
(20.183)

where

$$R_{\varphi} = e^{-i\vec{\sigma}\cdot\hat{n}\varphi/2} \tag{20.184}$$

and

 \hat{n} = unit vector in direction of axis of rotation φ = angle of rotation

We then assume that time-space components generate a rotation of the space axes with the time axis, which is a Lorentz transformation and that the operators in the new frame are given by

$$\vec{\sigma}' = L_v \vec{\sigma} L_v^{-1}, \ \vec{\alpha}' = L_v \vec{\alpha} L_v^{-1}, \ \beta' = L_v \beta L_v^{-1}$$
 (20.185)

where

$$L_v = e^{-i(i\vec{\alpha})\cdot\vec{\omega}/2} = e^{\vec{\alpha}\cdot\vec{\omega}/2} \to L_v^{-1} = e^{-\vec{\alpha}\cdot\vec{\omega}/2}$$
(20.186)

and

 $\vec{\omega}$ = vector in direction of velocity of primed frame

with respect to unprimed frame and of magnitude

$$\tanh(\omega) = \frac{v}{c}$$

Proof: First,

$$\sigma'_{\parallel} = L\sigma_{\parallel}L^{-1} = e^{\alpha_{\parallel}\omega/2}\sigma_{\parallel}e^{-\alpha_{\parallel}\omega/2} = e^{\alpha_{\parallel}\omega/2}e^{-\alpha_{\parallel}\omega/2}\sigma_{\parallel} = \sigma_{\parallel}$$
(20.187)

where we have used

$$\left[\alpha_{i},\sigma_{j}\right] = 2i\varepsilon_{ijk}\alpha_{k} \rightarrow \left[\alpha_{\parallel},\sigma_{\parallel}\right] = 0$$
(20.188)

This agrees with our earlier result.

Second,

$$\sigma'_{\perp} = L\sigma_{\perp}L^{-1} = e^{\alpha_{\parallel}\omega/2}\sigma_{\perp}e^{-\alpha_{\parallel}\omega/2} = e^{\alpha_{\parallel}\omega/2}e^{\alpha_{\parallel}\omega/2}\sigma_{\perp} = e^{\alpha_{\parallel}\omega}\sigma_{\perp} = e^{\vec{\alpha}\cdot\vec{\omega}}\sigma_{\perp}$$
(20.189)

where we have used

$$\{\alpha_i, \sigma_j\} = 0 \quad , \quad i \neq j \to \{\alpha_{\parallel}, \sigma_{\perp}\} = 0 \tag{20.190}$$

Now using $\vec{\omega} = \omega \hat{\omega}$, $\hat{\omega} \cdot \hat{\omega} = 1$ and $(\vec{\alpha} \cdot \hat{\omega})^2 = 1$ we get

$$e^{\vec{\alpha}\cdot\vec{\omega}} = \cosh\omega + \vec{\alpha}\cdot\hat{\omega}\sinh\omega \qquad (20.191)$$

This derivation is the analog of

$$e^{i\vec{\sigma}\cdot\hat{n}\theta} = \cos\theta + i\vec{\sigma}\cdot\hat{n}\sin\theta \qquad (20.192)$$

Therefore,

$$\sigma'_{\perp} = e^{\vec{\alpha} \cdot \vec{\omega}} \sigma_{\perp} = \cosh \omega \left[1 + \vec{\alpha} \cdot \hat{\omega} \tanh \omega \right] \sigma_{\perp} = \gamma \left[1 + \vec{\alpha} \cdot \hat{\omega} \tanh \omega \right] \sigma_{\perp}$$
(20.193)

where we have used

$$\cosh^2 \omega = \frac{1}{1 - \tanh^2 \omega} = \frac{1}{1 - (v/c)^2} = \gamma^2$$
 (20.194)

Using $\hat{\omega} \tanh \omega = \vec{v}/c$ we then get

$$\sigma'_{\perp} = \gamma \left[1 + \vec{\alpha} \cdot \hat{\omega} \tanh \omega \right] \sigma_{\perp} = \gamma \left[1 + \vec{\alpha} \cdot \vec{v}/c \right] \sigma_{\perp}$$
(20.195)

Finally, assuming $\vec{v} = v\hat{e}_z$ and using $\alpha_i \sigma_j = i\varepsilon_{ijk}\alpha_k$, $i \neq j$ we get

$$(\vec{\alpha} \cdot \vec{v}/c)\sigma_{\perp} = i\frac{\vec{v}}{c} \times \vec{\alpha}$$
(20.196)

so that

$$\sigma'_{\perp} = \gamma \left[\sigma_{\perp} + i \frac{\vec{v}}{c} \times \vec{\alpha} \right] \tag{20.197}$$

which agrees with our earlier result. Thus, $\vec{\sigma}$ transforms correctly. A similar calculation shows that $\vec{\alpha}$ transforms correctly also and, thus, our interpretation is correct.

What about the operator β ? In a new Lorentz frame we get

$$\beta' = L_v \beta L_v^{-1} = e^{\vec{\alpha} \cdot \vec{\omega}} \beta \tag{20.198}$$

since β anticommutes with $\vec{\alpha}$. We then get (as above)

$$\beta' = \gamma \left[\beta - (\vec{v}/c) \cdot \beta \vec{\alpha}\right] \tag{20.199}$$

where we have used $\beta \vec{\alpha} = -\vec{\alpha}\beta$. From the form of this transformation relation, it looks like β transforms as the time-component of a 4-vector of which $\beta \vec{\alpha}$ is the space part.

Some algebra shows that

$$\beta' \alpha_{\perp}' = L \beta \alpha_{\perp} L^{-1} = \beta \alpha_{\perp} \tag{20.200}$$

since both β and α_{\perp} anticommute with L and therefore $\beta \alpha_{\perp}$ commutes with L. In addition, we can show that

$$\beta' \alpha'_{\parallel} = \gamma \left[\beta \alpha_{\parallel} - (v/c) \beta \right]$$
(20.201)

Therefore, $(\beta, \beta \vec{\alpha})$ does transform like a 4-vector.

This 4-vector is called $\gamma^{\mu} = (\beta, \beta \vec{\alpha})$. In our earlier notation the space part is

$$\vec{\gamma} = \beta \vec{\alpha} = \begin{pmatrix} I & \vec{\tau} \\ -\vec{\tau} & I \end{pmatrix}$$
(20.202)

 $\vec{\gamma}$ is anti-Hermitian and γ^0 is Hermitian.

Some properties

$$(\gamma^0)^2 = 1$$
 , $(\gamma^i)^2 = -1$, $i = 1, 2, 3$ (20.203)

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 0 \quad , \quad \mu \neq \nu$$
 (20.204)

which are summarized by the relation

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu} \tag{20.205}$$

We also have

$$\sigma^{\mu\nu} = \frac{i}{2} \left[\gamma^{\mu}, \gamma^{\nu} \right] \tag{20.206}$$

In fact, any 4×4 matrix can be written as a unique linear combination of the γ^{μ} . The set of 16 matrices

$$I, \gamma^{\mu}, \sigma^{\mu\nu}, \gamma_5 \gamma^{\mu}, \gamma_5 \quad , \quad \text{where } \gamma_5 = \gamma^0 \gamma^1 \gamma^2 \gamma^3 \tag{20.207}$$

are linearly independent and complete. All are traceless except for the identity matrix.

The new operator γ_5 commutes with the γ^{μ} . This implies that it commutes with $\alpha_i = \gamma^0 \gamma^i$ and is invariant under a Lorentz transformation. It is not a scalar, however, since under parity

$$\beta \gamma_5 \beta = -\gamma_5 \tag{20.208}$$

This means that it is a *pseudoscalar*.

Similarly, $\gamma_5 \gamma^{\mu}$ is a *pseudovector* (or *axial vector*), which is a 4-vector whose space part does not change sign under parity and whose time component does.

We see that the set I, γ^{μ} , $\sigma^{\mu\nu}$, $\gamma_5\gamma^{\mu}$, γ_5 transforms as a scalar or zerothrank tensor, a vector or first-rank tensor, a second-rank tensor, a pseudovector or axial vector or a first-rank pseudotensor and a pseudoscalar or a zeroth-rank pseudotensor.

This is a clear indication that they are linearly independent.

20.6 The Dirac Equation

The scalar product of two 4-vectors is a Lorentz invariant. We have identified two 4-vectors, namely,

$$\gamma^{\mu} = (\beta, \beta \vec{\alpha}) \quad , \quad p^{\mu} = (E/c, \vec{p})$$
 (20.209)

Their scalar product is

$$\beta \frac{E}{c} - \beta \vec{\alpha} \cdot \vec{p} \tag{20.210}$$

Since it is an invariant, it has the same value in all frames. What is that value? We can find out by looking at its square

$$\left(\beta \frac{E}{c} - \beta \vec{\alpha} \cdot \vec{p}\right)^2 = \beta^2 \left(\frac{E}{c}\right)^2 + \left(\beta \vec{\alpha} \cdot \vec{p}\right)^2 - \beta \left(\beta \vec{\alpha} + \vec{\alpha} \beta\right) \cdot \frac{\vec{p}E}{c}$$
$$= \left(1\right) \left(\frac{E}{c}\right)^2 + \sum_i \left(\beta \alpha_i p_i\right)^2 - \beta \left(0\right) \cdot \frac{\vec{p}E}{c} = \left(\frac{E}{c}\right)^2 - \sum_i \left(\beta \alpha_i\right)^2 p_i^2$$
$$= \left(\frac{E}{c}\right)^2 - \sum_i \left(1\right)^2 p_i^2 = \left(\frac{E}{c}\right)^2 - p^2$$
(20.211)

This says that

$$\beta \frac{E}{c} - \beta \vec{\alpha} \cdot \vec{p} = \sqrt{\left(\frac{E}{c}\right)^2 - p^2} = \pm mc \qquad (20.212)$$

The sign depends on the sign we choose for β . If we had interpreted $\beta^2 = 1$ to mean $\beta = -1$ instead of +1, which is equivalent to choosing the parity operator as $-\beta$, no physics would have changed. This means we are free to choose the sign. We choose

$$\beta \frac{E}{c} - \beta \vec{\alpha} \cdot \vec{p} = +mc \tag{20.213}$$

or

$$\beta E - \beta c \vec{\alpha} \cdot \vec{p} = mc^2 \tag{20.214}$$

This operator equation involves 4×4 matrices which implies that any physical state vectors must be 4-component spinors.

We make the standard operator correspondence

$$E \to i\hbar \frac{\partial}{\partial t} \quad , \quad \vec{p} \to i\hbar \nabla$$
 (20.215)

and obtain a wave equation

$$i\hbar\beta\frac{\partial\psi}{\partial t} = \beta c\vec{\alpha} \cdot \frac{\hbar}{i}\nabla\psi + mc^2\psi \qquad (20.216)$$

or multiplying by β we get

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\vec{\alpha}\cdot\frac{\hbar}{i}\nabla + \beta mc^2\right]\psi \qquad (20.217)$$

which is the *Dirac equation* for a relativistic spin 1/2 particle.

The form of the result says that the Hamiltonian of a relativistic spin 1/2 particle is

$$\hat{H} = c\vec{\alpha} \cdot \vec{p} + \beta mc^2 \tag{20.218}$$

In the presence of an electromagnetic field we use minimal coupling to get

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\psi(\vec{r},t) = \left[c\vec{\alpha}\cdot\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right) + \beta mc^2\right]\psi(\vec{r},t)$$
(20.219)

We note that the vector potential \vec{A} (corresponding to spatial degrees of freedom) is directly coupled to $\vec{\alpha}$ corresponding to internal degrees of freedom).

20.6.1 Nonrelativistic Limit

First, we separate time using

$$\psi(t) = \psi e^{-iEt/\hbar} \tag{20.220}$$

to get

$$(E - e\Phi)\psi = \left[c\vec{\alpha} \cdot \left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right) + \beta mc^2\right]\psi \qquad (20.221)$$

We then write

$$\psi = \left(\begin{array}{c} \psi_A \\ \psi_B \end{array}\right) \tag{20.222}$$

where ψ_A and ψ_B are still two-component functions and use the explicit Dirac matrices to obtain

$$(E - e\Phi) \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \left[\begin{pmatrix} 0 & \vec{\tau} \\ \vec{\tau} & 0 \end{pmatrix} \cdot (c\vec{p} - e\vec{A}) + \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} mc^2 \right] \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} (20.223)$$

This is equivalent to two coupled equations

$$\vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right)\psi_B + mc^2\psi_A = (E - e\Phi)\psi_A \tag{20.224}$$

$$\vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right)\psi_A - mc^2\psi_B = (E - e\Phi)\psi_B \qquad (20.225)$$

Letting $E = E' + mc^2$ the second equation of the pair becomes

$$\psi_B = \frac{1}{E' - e\Phi + 2mc^2} \vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right) \psi_A \tag{20.226}$$

Inserting this result into the first equation of the pair we get

$$\frac{1}{2mc^2}\vec{\tau}\cdot\left(c\vec{p}-e\vec{A}\right)\frac{1}{1+\frac{E'-e\Phi}{2mc^2}}\vec{\tau}\cdot\left(c\vec{p}-e\vec{A}\right)\psi_A = \left(E'-e\Phi\right)\psi_A \tag{20.227}$$

These last two equations are exact and very useful substitutes for the Dirac equation.

We now make some approximations relevant to the nonrelativistic case. We assume that

$$E' << mc^2 \quad , \quad e\Phi << mc^2 \\ {\rm eigenvalues \ of \ } \vec{p} \ {\rm are \ of \ order \ } mv << mc \\$$

This says that the components satisfy

$$\psi_B \approx \frac{v}{c} \psi_A \tag{20.228}$$

Or that the 4-component wavefunction ψ has two large components ψ_A and two small components ψ_B .

If we ignore terms of order $(v/c)^2$ the equation for ψ_A becomes

$$\frac{1}{2mc^2} \left(\vec{\tau} \cdot \left(c\vec{p} - e\vec{A} \right) \right)^2 \psi_A + e\Phi\psi_A = E'\psi_A \tag{20.229}$$

Now, earlier we derived the identity

$$(\vec{\tau} \cdot \vec{a})(\vec{\tau} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\tau} \cdot \left(\vec{a} \times \vec{b}\right)$$
(20.230)

We then have

$$\left(\vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right)\right)^2 = \left(c\vec{p} - e\vec{A}\right)^2 + i\vec{\tau} \cdot \left(\left(c\vec{p} - e\vec{A}\right) \times \left(c\vec{p} - e\vec{A}\right)\right)$$
(20.231)

Now

$$\left(\vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right)\right)^2 = \left(c\vec{p} - e\vec{A}\right)^2 \tag{20.232}$$

and

$$(c\vec{p} - e\vec{A}) \times (c\vec{p} - e\vec{A}) = -ec(\vec{p} \times \vec{A} + \vec{A} \times \vec{p}) = +ie\hbar c(\nabla \times \vec{A} + \vec{A} \times \nabla) \quad (20.233)$$

Now

$$(\nabla \times \vec{A} + \vec{A} \times \nabla)^{i} \psi_{A} = \varepsilon^{ijk} (\partial_{j} A^{k} - A^{k} \partial_{j}) \psi_{A}$$

$$= \varepsilon^{ijk} ((\partial_{j} A^{k}) \psi_{A} + A^{k} (\partial_{j} \psi_{A}) - A^{k} (\partial_{j} \psi_{A}))$$

$$= \varepsilon^{ijk} (\partial_{j} A^{k}) \psi_{A} = (\nabla \times \vec{A}) \psi_{A} = \vec{B} \psi_{A}$$
(20.234)

Putting everything together we get

$$\frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2\psi_A - \frac{e}{mc}\frac{\hbar}{2}\vec{\tau}\cdot\vec{B} + e\Phi\psi_A = E'\psi_A \qquad (20.235)$$

This the *Pauli equation*. The term involving the magnetic field has the form of a magnetic dipole interaction energy

$$-\frac{e}{mc}\vec{S}\cdot\vec{B} \tag{20.236}$$

with a gyromagnetic ratio

$$2 \times \frac{e}{mc} \to g = 2 \tag{20.237}$$

The full time-dependent form of the nonrelativistic limit is given by

$$\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}\right)^2 \psi_A - \frac{e}{mc} \frac{\hbar}{2} \vec{\tau} \cdot \vec{B} + (e\Phi + mc^2) \psi_A = i\hbar \frac{\partial \psi_A}{\partial t}$$
(20.238)

20.6.2 Currents and Continuity Equations

Going back to the full equation

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\psi(\vec{r},t) = \left[c\vec{\alpha}\cdot\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right) + \beta mc^2\right]\psi(\vec{r},t)$$
(20.239)

we take the Hermitian conjugate to get

$$\left(-i\hbar\frac{\partial}{\partial t} - e\Phi\right)\psi^{+}(\vec{r},t) = c\left(-\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\psi^{+}(\vec{r},t)\cdot\vec{\alpha} + \beta mc^{2}\psi^{+}(\vec{r},t) \quad (20.240)$$

Note that the Hermitian conjugate operation reverses matrix order. Now multiply the first equation by $\psi^+(\vec{r},t)$ on the left and the second equation by $\psi(\vec{r},t)$ on the right and subtracting we get the continuity-type equation

$$\frac{\partial \left(\psi^{+}\psi\right)}{\partial t} + \nabla \cdot \left(\psi^{+}c\vec{\alpha}\psi\right) = 0$$
(20.241)

This says that the quantity $\psi^+\psi$ is a positive conserved quantity that can be interpreted as a probability density and then

$$\vec{j} = \psi^+ c \vec{\alpha} \psi \tag{20.242}$$

is the corresponding probability current. The operator $c\vec{\alpha}$ corresponds to the velocity operator, which is the derivative of the Hamiltonian with respect to \vec{p} .

What happens to the Dirac equation under a Lorentz transformation?

In one frame we have

$$i\hbar\beta\frac{\partial\psi}{\partial t} = \beta c\vec{\alpha} \cdot \frac{\hbar}{i}\nabla\psi + mc^2\psi \qquad (20.243)$$

and in a new frame we have

$$i\hbar\beta'\frac{\partial\hat{\psi}(\vec{r}\,',t')}{\partial t'} = \beta'c\vec{\alpha}\,'\cdot\frac{\hbar}{i}\nabla'\hat{\psi}(\vec{r}\,',t') + mc^2\hat{\psi}(\vec{r}\,',t') \tag{20.244}$$

where $\hat{\psi}(\vec{r}',t')$ is the wave function in the new frame.

We already determined, however, that

$$i\hbar\beta'\frac{\partial}{\partial t'} - \beta'c\vec{\alpha}' \cdot \frac{\hbar}{i}\nabla' = i\hbar\beta\frac{\partial}{\partial t} - \beta c\vec{\alpha} \cdot \frac{\hbar}{i}\nabla \qquad (20.245)$$

since the scalar product of two 4-vectors is an invariant. This implies that

$$\hat{\psi}(\vec{r}',t') = \psi(\vec{r},t) = \text{Lorentz scalar}$$
 (20.246)

i.e., they both satisfy the same equation when \vec{r}', t' and \vec{r}, t are the same spacetime point.

It turns out, however, that a more convenient equation to use in the new frame is one that still involves the old β and $\vec{\alpha}$ matrices, i.e., β' and $\vec{\alpha}'$ are represented by the same matrices as β and $\vec{\alpha}$. We can find this other equation as follows. We have

$$\begin{split} i\hbar\beta'\frac{\partial\hat{\psi}(\vec{r}\,',t')}{\partial t'} &=\beta'c\vec{\alpha}\,'\cdot\frac{\hbar}{i}\nabla'\hat{\psi}(\vec{r}\,',t')+mc^{2}\hat{\psi}(\vec{r}\,',t')\\ i\hbar L_{v}\beta L_{v}^{-1}\frac{\partial\hat{\psi}(\vec{r}\,',t')}{\partial t'} &=L_{v}\beta c\vec{\alpha}L_{v}^{-1}\cdot\frac{\hbar}{i}\nabla'\hat{\psi}(\vec{r}\,',t')+mc^{2}\hat{\psi}(\vec{r}\,',t')\\ i\hbar\beta L_{v}^{-1}\frac{\partial\hat{\psi}(\vec{r}\,',t')}{\partial t'} &=\beta c\vec{\alpha}L_{v}^{-1}\cdot\frac{\hbar}{i}\nabla'\hat{\psi}(\vec{r}\,',t')+mc^{2}L_{v}^{-1}\hat{\psi}(\vec{r}\,',t') \end{split}$$

If we define

$$\psi'(\vec{r}\,',t') = L_v^{-1}\hat{\psi}(\vec{r}\,',t') = L_v^{-1}\psi(\vec{r},t)$$
(20.247)

we have the equation

$$i\hbar\beta \frac{\partial\psi'(\vec{r}\,',t')}{\partial t'} = \beta c\vec{\alpha} \cdot \frac{\hbar}{i} \nabla'\psi'(\vec{r}\,',t') + mc^2\psi'(\vec{r}\,',t')$$
(20.248)

This form of the equation has the same matrices β and $\vec{\alpha}$ in all frames with the wave function in the new frame related to the wave function in the old frame by the Lorentz transformation.

Alternatively, we can write the Dirac equation in covariant form. The Dirac equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\vec{\alpha}\cdot\frac{\hbar}{i}\nabla + \beta mc^2\right]\psi \qquad (20.249)$$

which we can rewrite as

$$-i\hbar\beta\partial_0\psi - i\hbar\beta\alpha^i\partial_i\psi + mc\psi = 0 \tag{20.250}$$

using the definition of the Dirac gamma matrices we have

$$\left(-i\gamma^{\mu}\partial_{\mu} + \frac{mc}{\hbar}\right)\psi = 0 \tag{20.251}$$

which is clearly covariant.

20.6.3 Free Particle Solutions

We start off by constructing solutions for a particle at rest. In this case, we have

$$\psi(\vec{r},t) = e^{-iEt/\hbar}u \tag{20.252}$$

where u is a spinor independent of space and time. Substituting into the Dirac equation we have

$$Eu = \beta mc^2 u \tag{20.253}$$

The eigenvalues of β are ± 1 . If u is an eigenstate of β with eigenvalue +1, then $E = +mc^2$ and if u is an eigenstate of β with eigenvalue -1, then $E = -mc^2$. So we find negative energy solutions again and we will associate them with particles and antiparticles as before. Their properties in the spin 1/2 case will be different, however.

We choose to write four linearly independent solutions to the free particle Dirac equation as:

$$u_{0\uparrow}^{(+)} = \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix} , \quad u_{0\downarrow}^{(+)} = \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix} , \quad u_{0\downarrow}^{(-)} = \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix} , \quad u_{0\uparrow}^{(-)} = \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}$$

where the upper index (\pm) denotes the eigenvalue of β , the 0 denotes that the particle is at rest $\vec{p} = 0$, and the arrow denotes the value of the spin associated physically with these states.

The spinors $u_{0\uparrow}^{(+)}$ and $u_{0\downarrow}^{(-)}$ are eigenstates of σ_z with eigenvalue +1 and $u_{0\downarrow}^{(+)}$ and $u_{0\uparrow}^{(-)}$ are eigenstates of σ_z with eigenvalue -1.

We are saying here that while $u_{0\uparrow}^{(-)}$ is the spinor of a negative energy particle with spin up, we will associate it with a positive energy antiparticle with spin down.

The states with $\beta = +1$ vary in time as $e^{-imc^2t/\hbar}$ and those with $\beta = -1$ vary in time as $e^{+imc^2t/\hbar}$. The positive and negative states have opposite parity(intrinsic).

We can now construct states for a particle with momentum \vec{p} by starting with

the particle at rest and applying a Lorentz transformation to take us to a frame moving with velocity

$$\vec{v} = -\frac{\vec{p}c^2}{E_p}$$
 where $E_p = +\sqrt{p^2c^2 + m^2c^4}$ (20.254)

We showed earlier that

$$\psi'(\vec{r}\,',t') = L_v^{-1}\psi(\vec{r},t) = e^{-\vec{\alpha}\cdot\vec{\omega}/2}\psi(\vec{r},t) = e^{-\vec{\alpha}\cdot\vec{\omega}/2}e^{\mp imc^2t/\hbar}u_{0,\sigma}^{(\pm)}$$
(20.255)

Now $E'_p t' - \vec{p}' \cdot \vec{r}'$ is a Lorentz scalar (scalar product of two 4-vectors). In the rest frame it is equal to mc^2t . Therefore we can write

$$e^{\pm imc^2 t/\hbar} = e^{\pm i(\vec{p}' \cdot \vec{r}\,' - E'_p t')/\hbar} \tag{20.256}$$

Dropping the superfluous primes we then have

$$\psi(\vec{r},t) = e^{\pm i(\vec{p}\cdot\vec{r}-E_pt)/\hbar} e^{-\vec{\alpha}\cdot\vec{\omega}/2} u_{0,\sigma}^{(\pm)}$$
(20.257)

as the wave function for nonzero momentum. The new spinors are given by

$$u_{\vec{p},\sigma}^{(\pm)} = e^{-\vec{\alpha}\cdot\vec{\omega}/2} u_{0,\sigma}^{(\pm)} = \left[\cosh\frac{\omega}{2} - \vec{\alpha}\cdot\hat{v}\sinh\frac{\omega}{2}\right] u_{0,\sigma}^{(\pm)}$$
(20.258)

Using

$$\vec{v} = -\frac{\vec{p}c^2}{E_p} \tag{20.259}$$

we get

$$\cosh \frac{\omega}{2} = \sqrt{\frac{E_p + mc^2}{2mc^2}} , \quad \hat{v} \tanh \frac{\omega}{2} = -\frac{\vec{p}c}{E_p + mc^2}$$
(20.260)

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so that

$$u_{\vec{p},\sigma}^{(\pm)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \left[1 + \frac{c\vec{p} \cdot \vec{\alpha}}{E_p + mc^2} \right] u_{0,\sigma}^{(\pm)}$$
(20.261)

We then have (in the standard representation)

$$u_{\vec{p},\uparrow}^{(+)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \left[1 + \frac{c}{E_p + mc^2} \vec{p} \cdot \vec{\alpha} \right] u_{0,\uparrow}^{(+)}$$
(20.262)

Now

$$\begin{split} \vec{p} \cdot \vec{\alpha} &= p_x \left(\begin{array}{cccc} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{array} \right) + p_y \left(\begin{array}{cccc} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{array} \right) \\ &+ p_z \left(\begin{array}{cccc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{array} \right) \quad , \quad u_{0,\uparrow}^{(+)} = \left(\begin{array}{c} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{array} \right) \end{split}$$

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and we get

$$\begin{split} u_{\vec{p},\uparrow}^{(+)} &= \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{bmatrix} \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix} \\ &+ \frac{c}{E_p + mc^2} \begin{pmatrix} p_x \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix} + p_y \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix} + p_z \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix} \end{pmatrix} \\ &= \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} 1\\0\\\frac{cp_z}{E_p + mc^2}\\\frac{c(p_x + ip_y)}{E_p + mc^2} \end{pmatrix} \end{split}$$
(20.263)

and similarly

$$u_{\vec{p},\downarrow}^{(+)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} 0\\1\\\frac{c(p_x - ip_y)}{E_p + mc^2}\\-\frac{cp_z}{E_p + mc^2} \end{pmatrix}$$
(20.264)
$$u_{\vec{p},\downarrow}^{(-)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} \frac{cp_x - ip_y}{E_p + mc^2}\\1\\0 \end{pmatrix}$$
(20.265)
$$u_{\vec{p},\uparrow}^{(-)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} \frac{c(p_x - ip_y)}{E_p + mc^2}\\-\frac{cp_z}{E_p + mc^2}\\0\\1 \end{pmatrix}$$
(20.266)

Remember that the arrow refers to the spin associated with the state in the rest frame, which is minus the σ_z eigenvalue for the (-) spinors. We see that a particle in a σ_z eigenstate in its rest frame appears to be in a σ_z eigenstate to an observer moving with respect to the particle only if the observer is moving along the z-direction, i.e., if $p_x = p_y = 0$ we have

$$u_{\vec{p},\uparrow}^{(+)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} 1\\ 0\\ \frac{cp_z}{E_p + mc^2}\\ 0 \end{pmatrix} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \left[u_{0,\uparrow}^{(+)} + \frac{cp_z}{E_p + mc^2} u_{0,\downarrow}^{(-)} \right] (20.267)$$

which is a sum of a particle and an antiparticle where both have spin up!

The positive energy solutions $u_{\vec{p}\sigma}^{(+)}e^{i(\vec{p}\cdot\vec{r}-E_pt)/\hbar}$ correspond to particles with momentum \vec{p} , energy E_p and spin orientation σ . The negative energy solutions

 $u_{\vec{p}\sigma}^{(-)}e^{-i(\vec{p}\cdot\vec{r}-E_pt)/\hbar}$ correspond to particles with momentum $-\vec{p}$, energy $-E_p$ and spin orientation $-\sigma$ which we will soon associate with antiparticles with momentum \vec{p} , energy E_p and spin orientation σ .

The nonzero momentum spinors are orthogonal but not normalized to one (as is the case with the zero momentum spinors). Since $L^+ \neq L^{-1}$, in general, the Lorentz transformations are not represented by a unitary operator and hence the lengths of vectors or normalizations change. In particular. The normalization is given by

$$u_{\vec{p}\sigma}^{(\pm)+}u_{\vec{p}\sigma}^{(\pm)} = \frac{E_p}{mc^2}$$
(20.268)

Since $\vec{\alpha}$ is Hermitian, we have $L^+ = L$.

Thus, if
$$u_{\vec{p}} = L^{-1}u_0$$
, then $(u_{\vec{p}})^+ = (u_0)^+ (L^{-1})^+ = (u_0)^+ L^{-1}$ and $u_{\vec{p}}^+ u_{\vec{p}} = u_0^+ (L^{-1})^2 u_0$

It is possible to define a normalization that is invariant under a Lorentz transformation. Since β anticommutes with $\vec{\alpha}$, we can write

$$(L^{-1})^{+}\beta = L^{-1}\beta = e^{\vec{\alpha}\cdot\vec{\omega}/2}\beta = \beta e^{-\vec{\alpha}\cdot\vec{\omega}/2} = \beta L$$
(20.269)

Now, if the spinor u transforms as $u'=L^{-1}u,$ then the spinor $\bar{u}=u^+\beta$ is given in the new frame by

$$\bar{u}' = u'^{+}\beta' = u'^{+}\beta = u^{+}(L^{-1})^{+}\beta = u^{+}L^{-1}\beta = u^{+}\beta L = \bar{u}L$$
(20.270)

This means that the product $\bar{u}_1 u_2$ of any two spinors is a Lorentz invariant, i.e.,

$$\bar{u}_1' u_2' = (\bar{u}_1 L) (L^{-1} u_2) = \bar{u}_1 u_2$$
(20.271)

In the rest frame

$$u_{0\sigma}^{(b)+}u_{0\sigma'}^{(b')} = b\delta_{bb'}\delta_{\sigma\sigma'} \quad , \quad b = \pm$$
(20.272)

which says that the same relation is true for all momentum \vec{p}

$$u_{\vec{p}\sigma}^{(b)+}u_{\vec{p}\sigma'}^{(b')} = b\delta_{bb'}\delta_{\sigma\sigma'} \quad , \quad b = \pm$$
(20.273)

The spinors $u_{\vec{p}\sigma}^{(\pm)}$ obey the completeness relation that says that the 4×4 identity matrix can be written as the sum of the outer products of the four spinors, i.e.,

$$\sum_{b,\sigma} b u^{(b)}_{\vec{p}\sigma} \bar{u}^{(b)}_{\vec{p}\sigma} = 1$$
(20.274)

The spinors $u_{\vec{p}\sigma}^{(\pm)}$ obey

$$(\beta E_p - c\beta \vec{\alpha} \cdot \vec{p}) u_{\vec{p}\sigma}^{(\pm)} = \pm m c^2 u_{\vec{p}\sigma}^{(\pm)}$$

$$(20.275)$$

and

$$u_{\vec{p}\sigma}^{(\pm)+}(\beta E_p - c\vec{\alpha} \cdot \vec{p}\beta) = \pm mc^2 u_{\vec{p}\sigma}^{(\pm)+}$$
(20.276)

Multiplying the last equation on the right by β we have the equation satisfied by $\bar{u}_{\vec{v}\sigma}^{(\pm)}$

$$\bar{u}_{\vec{p}\sigma}^{(\pm)}(\beta E_p - c\beta\vec{\alpha}\cdot\vec{p}) = \pm mc^2 \bar{u}_{\vec{p}\sigma}^{(\pm)}$$
(20.277)

20.6.4 More About Currents

As we have seen, the solution of the Dirac equation $\psi(\vec{r},t)$ has the following behavior under a Lorentz transformation

$$\psi(\vec{r},t) \to \psi'(\vec{r}',t') = L^{-1}\psi(\vec{r},t)$$
 (20.278)

The spinor $\bar{\psi}(\vec{r},t) = \psi^+(\vec{r},t)\beta$ transforms like

$$\bar{\psi}(\vec{r},t) \to \bar{\psi}'(\vec{r}',t') = [L^{-1}\psi(\vec{r},t)]^+ \beta = \bar{\psi}(\vec{r},t)L$$
 (20.279)

This says that the product $\bar{\psi}(\vec{r},t)\psi(\vec{r},t)$ transforms like a Lorentz scalar.

Now the γ^{μ} transform as the components of a 4-vector, i.e., $\gamma^{\mu} \to L \gamma^{\mu} L^{-1}$. Therefore, the product

$$\bar{\psi}(\vec{r},t)\gamma^{\mu}\psi(\vec{r},t) = \left(\rho(\vec{r},t), \frac{1}{c}\vec{j}(\vec{r},t)\right)$$
(20.280)

transforms like a 4-vector under a Lorentz transformation. It is the particle 4-current multiplied by 1/c. In the same manner,

 $\bar{\psi}\sigma^{\mu\nu}\psi \rightarrow \text{ second -rank tensor}$ $\bar{\psi}\gamma_5\gamma^{\mu}\psi \rightarrow \text{ axial vector}$ $\bar{\psi}\gamma_5\psi \rightarrow \text{ pseudo - scalar}$

The positive density $\rho(\vec{r},t) = \psi^+(\vec{r},t)\psi(\vec{r},t)$ and the current $\vec{j}(\vec{r},t) = c\psi^+(\vec{r},t)\vec{\alpha}\psi(\vec{r},t)$ satisfy the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0 \tag{20.281}$$

which implies that the quantity

$$\int \rho(\vec{r},t)d^3r \tag{20.282}$$

is a constant of the motion.

In this case, we can interpret $\rho(\vec{r},t)$ as a probability density (same as in non-relativistic case). Remember in the spin zero case this was not so since the corresponding conserved density needed to be interpreted as a charge density which could be positive and negative.

One important consequence in the spin zero case was that it is impossible for a particle to make a transition from a state normalized to +1 to a state normalized to -1 since the normalization remains constant in time. We associated the negative energy states with particles and the negatively normalized states with antiparticles. We then see that the impossibility of a transition between positive and negative energy states just corresponds to charge conservation.

In the spin-1/2 case, however, both positive and negative energy states have positive normalization so that there is nothing in the theory (so far) that prevents a particle in a positive energy state from making a transition to a negative energy state radiating away several high energy photons in the process. A difficulty in the theory that we must return to later!

Let us say some more about the position and velocity operators in the Dirac theory.

The position operator has strange features similar to those of the Klein-Gordon theory. If we apply the position operator to a wave packet made up of positive energy free particle states we get

$$\vec{r}\psi^{(+)}(\vec{r}) = \vec{r}\left(\sum_{\sigma} \int \frac{d^3p}{(2\pi\hbar)^3} a_{\vec{p}\sigma} u^{(+)}_{\vec{p}\sigma} e^{i\vec{p}\cdot\vec{r}/\hbar}\right) = \sum_{\sigma} \int \frac{d^3p}{(2\pi\hbar)^3} a_{\vec{p}\sigma} u^{(+)}_{\vec{p}\sigma} \frac{\hbar}{i} \nabla_{\vec{p}} e^{i\vec{p}\cdot\vec{r}/\hbar}$$
$$= \sum_{\sigma} \int \frac{d^3p}{(2\pi\hbar)^3} (i\hbar\nabla_{\vec{p}} a_{\vec{p}\sigma}) u^{(+)}_{\vec{p}\sigma} e^{i\vec{p}\cdot\vec{r}/\hbar} + \sum_{\sigma} \int \frac{d^3p}{(2\pi\hbar)^3} a_{\vec{p}\sigma} (i\hbar\nabla_{\vec{p}} u^{(+)}_{\vec{p}\sigma}) e^{i\vec{p}\cdot\vec{r}/\hbar}$$

where we have integrated by parts to get the last two terms. The first term contains only positive energy components. The second term, however, contains the factor $i\hbar\nabla_{\vec{p}}u_{\vec{p}\sigma}^{(+)}$, which generates both positive and negative components (explicitly do the derivatives on the column vectors we derived earlier). If we define, as before

$$\vec{r} = \vec{r}_{(+)} + \vec{r}_{(-)} \tag{20.283}$$

then, as before, the even part $\vec{r}_{(+)}$ acting on the wave packet of positive energy free particle states produces only positive energy free particle states and acting on the wave packet of negative energy free particle states produces only negative energy free particle states, while the odd part $\vec{r}_{(-)}$ turns positive positive energy states to negative energy states and vice versa.

As in the Klein-Gordon case, both positive and negative energy free particle solutions are needed to produce a localized wave packet.

Looking at the current expression $\vec{j}(\vec{r},t) = c\psi^+(\vec{r},t)\vec{\alpha}\psi(\vec{r},t)$ we see that the operator $c\vec{\alpha}$ acts as a velocity operator. This interpretation also agrees with the commutator relation

$$-i\hbar\left[\vec{r},\hat{H}\right] = c\vec{\alpha} \tag{20.284}$$

which leads to the Heisenberg representation operator equation

$$\frac{d\vec{r}}{dt} = c\vec{\alpha} \tag{20.285}$$

If, however, we consider the z-component of this velocity operator we get $(c\alpha_z)^2 = c^2 \alpha_z^2 = c^2$. Thus the eigenvalues of each component of the velocity

operator are $\pm c$, which says that a particle in an eigenstate of the velocity operator travels at the speed of light!

This means that the velocity operator is not simply related to the momentum operator relativistically. The eigenstates of any component of $\vec{\alpha}$ are linear combinations of positive and negative energy free particle states and thus cannot be realized in any physical situation! For any arbitrary state the expectation value of $c\vec{\alpha}$ has a magnitude between 0 and c.

20.6.5 Non-relativistic Limit

We now derive corrections to the Pauli equation. Earlier we had

$$\vec{\tau} \cdot (c\vec{p} - e\vec{A})\psi_B + mc^2\psi_A = (E - e\Phi)\psi_A \qquad (20.286)$$

$$\vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right)\psi_A - mc^2\psi_B = (E - e\Phi)\psi_B \qquad (20.287)$$

or

$$\vec{\tau} \cdot \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}\right) \psi_B + mc \psi_A = \frac{1}{c} \left(i\hbar \frac{\partial}{\partial t} - e\Phi\right) \psi_A \tag{20.288}$$

$$\vec{\tau} \cdot \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}\right) \psi_A - mc \psi_B = \frac{1}{c} \left(i\hbar \frac{\partial}{\partial t} - e\Phi\right) \psi_B \tag{20.289}$$

The second equation of the above pair gives (an exact equation)

$$\psi_B = \frac{1}{2mc} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right) \cdot \vec{\tau} \psi_A - \frac{1}{2mc^2} \left(i\hbar \frac{\partial}{\partial t} - mc^2 - e\Phi \right) \psi_B$$
(20.290)

Now the ψ_A term is much larger than the ψ_B term on the right. Thus, we get the first correction by iterating once, i.e.

$$\psi_B = \frac{1}{2mc} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right) \cdot \vec{\tau} \psi_A - \frac{1}{4m^2 c^3} \left(i\hbar \frac{\partial}{\partial t} - mc^2 - e\Phi \right) \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right) \cdot \vec{\tau} \psi_A$$
(20.291)

Substituting this expression into the first equation of the pair we get the first relativistic correction term to the Pauli equation

$$-\frac{1}{4m^2c^3}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right) \cdot \vec{\tau}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right) \cdot \vec{\tau}\psi_A \qquad (20.292)$$

which is $\approx (v/c)^2$ smaller than the kinetic energy term $p^2/2m$.

The correction term can be rewritten as

$$-\frac{1}{4m^2c^3}\left(\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\cdot\vec{\tau}\right)^2\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)\psi_A \\ -\frac{ie\hbar}{4m^2c^3}\left(\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\cdot\vec{\tau}\right)(\vec{\varepsilon}\cdot\vec{\tau})\psi_A$$

where

$$\vec{\varepsilon} = -\nabla \Phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} = \text{ electric field}$$
 (20.293)

To lowest order in (v/c) we have

$$\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)\psi_A = \frac{p^2}{2m}\psi_A \tag{20.294}$$

Using this relation with the identity

$$(\vec{\tau} \cdot \vec{a})(\vec{\tau} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\tau} \cdot \left(\vec{a} \times \vec{b}\right)$$
(20.295)

the correction becomes

$$-\left[\frac{p^4}{8m^3c^2} + \frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot(\vec{\varepsilon}\times\vec{p}) + \frac{ie\hbar}{4m^2c^2}\vec{p}\cdot\vec{\varepsilon}\right]$$
(20.296)

The first term is the relativistic correction to the kinetic energy. The second term is the spin-orbit coupling. The third term is new and is not even Hermitian!

The reason for this non-Hermitian term is that we are only working to order $(v/c)^2$. Such a non-Hermitian term in the wave equation means that the normalization integral

$$\int \psi_A^+ \psi_A d^3 r$$

can change in time. Now the full Dirac equation obeys the normalization condition

$$\int \psi^{+} \psi d^{3}r = \int \left[\psi_{A}^{+} \psi_{A} + \psi_{B}^{+} \psi_{B}\right] d^{3}r = 1$$
(20.297)

To lowest order, however,

$$\psi_B = \frac{\hbar}{2imc} \nabla \cdot \vec{\tau} \psi_A \to \psi_B^+ \psi_B = \psi_A^+ \frac{p^2}{4m^2c^2} \psi_A \qquad (20.298)$$

Thus, the integral stays constant to order $(v/c)^2$. It is the integral

$$\int \psi_A^+ \left[1 + \frac{p^2}{4m^2c^2} \right] \psi_A d^3 r = \int \left[\left[1 + \frac{p^2}{8m^2c^2} \right] \psi_A \right]^+ \left[\left[1 + \frac{p^2}{8m^2c^2} \right] \psi_A \right] d^3 r$$

to order $(v/c)^2$, that remains constant and equal to 1. This implies that the correct nonrelativistic limit of the Dirac wave function (the limit whose normalization remains constant in time) is

$$\psi(\vec{r},t) = \left[1 + \frac{p^2}{8m^2c^2}\right]\psi_A(\vec{r},t) \to \int \psi^+ \psi d^3r = 1$$
(20.299)

The equation for this form of the wave function will not have any non-Hermitian terms. A large amount of algebra gives the equation for $\psi(\vec{r}, t)$ as

$$i\hbar\frac{\partial\psi}{\partial t} = \left[mc^2 + \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \frac{p^4}{8m^3c^2}\right]\psi$$

$$-\left[\frac{e\hbar}{2mc}\vec{\tau}\cdot\vec{B} + \frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot(\vec{\varepsilon}\times\vec{p})\right]\psi + \left[e\Phi + \frac{\hbar^2}{8m^2c^2}(\nabla^2 e\Phi)\right]$$
(20.300)

This is the correct nonrelativistic limit of the Dirac equation. All terms are Hermitian.

The terms on the right-hand side are

[rest energy + kinetic energy(to order $(v/c)^2$)]

- [Pauli magnetic moment energy + spin-orbit energy]
- + [correction to the potential energy term]

Spin-Orbit Term - Letting $\vec{A} = 0$ for simplicity we have

$$\frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot\left(\vec{\varepsilon}\times\vec{p}\right) = -\frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot\left(\nabla\Phi\times\vec{p}\right)$$
(20.301)

If we assume the potential is spherically symmetric, then

$$\nabla \Phi = \frac{1}{r} \frac{d\Phi}{dr} \vec{r} \tag{20.302}$$

and we get

$$\frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot(\vec{\varepsilon}\times\vec{p}) = -\frac{e\hbar}{4m^2c^2r}\frac{d\Phi}{dr}\vec{\tau}\cdot(\vec{r}\times\vec{p}) = -\frac{e}{2m^2c^2r}\frac{d\Phi}{dr}\vec{S}\cdot\vec{L}$$
(20.303)

which is the spin-orbit energy. It correctly contains the Thomas precession correction! We do not have to add any terms in an ad hoc manner!

Correction to the Potential - This is called the *Darwin term*. Now, from Poisson's equation we have

$$\nabla^2 e \Phi(\vec{r}) = -4\pi e Q(\vec{r})$$
, $Q(\vec{r}) = \text{charge density producing } \Phi(\vec{r})$

For a Coulomb potential we get

$$\frac{\hbar^2}{8m^2c^2}(\nabla^2 e\Phi) = \frac{\pi\hbar^2}{2m^2c^2}Ze^2\delta(\vec{r})$$
(20.304)

This term tends to raise the energy of s-states since they do not vanish at the origin.

20.6.6 The Dirac Hydrogen Atom

We start with the equations

$$\vec{\sigma} \cdot \left(c\vec{p} - e\vec{A}\right)\psi_B + mc^2\psi_A = (E - e\Phi)\psi_A \tag{20.305}$$

$$\vec{\sigma} \cdot (c\vec{p} - e\vec{A})\psi_A - mc^2\psi_B = (E - e\Phi)\psi_B \qquad (20.306)$$

where we have substituted $\vec{\sigma}$ for $\vec{\tau}$. The potential function is $e\Phi = -Ze^2/r$ and we let $\vec{A} = 0$. Writing

$$\psi_A = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} , \quad \psi_B = \begin{pmatrix} u_3 \\ u_4 \end{pmatrix}$$
(20.307)

we get

$$-\frac{i}{\hbar c}\left[E + \frac{Ze^2}{r} - mc^2\right]u_1 + \frac{\partial u_4}{\partial x} - i\frac{\partial u_4}{\partial y} + \frac{\partial u_3}{\partial z} = 0$$
(20.308)

$$-\frac{i}{\hbar c} \left[E + \frac{Ze^2}{r} - mc^2 \right] u_2 + \frac{\partial u_3}{\partial x} + i \frac{\partial u_3}{\partial y} - \frac{\partial u_4}{\partial z} = 0$$
(20.309)

$$-\frac{i}{\hbar c} \left[E + \frac{Ze^2}{r} + mc^2 \right] u_3 + \frac{\partial u_2}{\partial x} - i\frac{\partial u_2}{\partial y} + \frac{\partial u_2}{\partial z} = 0$$
(20.310)

$$-\frac{i}{\hbar c} \left[E + \frac{Ze^2}{r} + mc^2 \right] u_4 + \frac{\partial u_1}{\partial x} + i \frac{\partial u_1}{\partial y} - \frac{\partial u_2}{\partial z} = 0$$
(20.311)

We now use another clever trick I learned from Professor Hans Bethe at Cornell University to find a solution.

If we consider only large components, i.e., set the small components to zero, then $[\vec{L}, \hat{H}]$, which is proportional to $\vec{\alpha} \times \vec{p}$, will be zero, since $\vec{\alpha}$ connects the small and large components. This means that ψ_A will be an eigenfunction of \vec{L} . In addition, it must contain one spin component with spin up and another with spin down.

Of course, \vec{j} and j_z are constants of the motion. Hence, for $j=\ell+1/2$ we can set

$$u_1 = g(r) \sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}} Y_{\ell}^{m - \frac{1}{2}}(\Omega)$$
(20.312)

$$u_2 = -g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}}Y_{\ell}^{m + \frac{1}{2}}(\Omega)$$
(20.313)

where the unknown function g(r) will be the solution of some relativistic radial equation.

To get the small components we recall the equation

$$\psi_B = \frac{1}{E' - e\Phi + 2mc^2} \vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right) \psi_A \tag{20.314}$$

and note that the operator which gives the small component from the large component has odd parity (\vec{p} is odd, $\vec{A} = 0$ and everything else is even) and commutes with \vec{j} . Hence, ψ_B must belong to the same j value as ψ_A but must have a different ℓ .

Corresponding to $j = \ell + 1/2$ the only other possible value of the orbital angular momentum is $\ell' = \ell + 1$. Therefore, we set (remembering the appropriate Clebsch-Gordon coefficients)

$$u_{3} = if(r)\sqrt{\frac{\ell - m + \frac{3}{2}}{2\ell + 3}}Y_{\ell+1}^{m-\frac{1}{2}}(\Omega)$$
(20.315)

$$u_4 = -if(r)\sqrt{\frac{\ell+m+\frac{3}{2}}{2\ell+3}}Y_{\ell+1}^{m+\frac{1}{2}}(\Omega)$$
(20.316)

where the unknown function f(r) will be the solution of some relativistic radial equation. Inserting these solution guesses into the 4 coupled equations we find that for $j = \ell + 1/2$ the connection between f and g is given by

$$\frac{1}{\hbar c} \left[E + \frac{Ze^2}{r} + mc^2 \right] f = \frac{dg}{dr} - \ell \frac{g}{r}$$
(20.317)

$$\frac{1}{hc} \left[E + \frac{Ze^2}{r} - mc^2 \right] g = -\frac{df}{dr} - (\ell + 2)\frac{f}{r}$$
(20.318)

In an analogous way for $j = \ell - 1/2$ we have

$$u_{1} = g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}}Y_{\ell}^{m - \frac{1}{2}}(\Omega)$$
(20.319)

$$u_2 = g(r) \sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}} Y_{\ell}^{m + \frac{1}{2}}(\Omega)$$
(20.320)

$$u_{3} = -if(r)\sqrt{\frac{\ell + m - \frac{1}{2}}{2\ell - 1}}Y_{\ell-1}^{m-\frac{1}{2}}(\Omega)$$
(20.321)

$$u_4 = if(r)\sqrt{\frac{\ell - m - \frac{1}{2}}{2\ell - 1}}Y_{\ell-1}^{m+\frac{1}{2}}(\Omega)$$
(20.322)

and

$$\frac{1}{\hbar c} \left[E + \frac{Ze^2}{r} + mc^2 \right] f = \frac{dg}{dr} + (\ell + 1)\frac{g}{r}$$
(20.323)

$$\frac{1}{\hbar c} \left[E + \frac{Ze^2}{r} - mc^2 \right] g = -\frac{df}{dr} + (\ell - 1)\frac{f}{r}$$
(20.324)

We now define

$$k = \begin{cases} -(\ell+1) & \text{if } j = \ell + 1/2 \\ \ell & \text{if } j = \ell + 1/2 \end{cases}$$
(20.325)

i.e.,

$$k = \begin{cases} -1, -2, \dots & \text{if } j = \ell + 1/2 \\ 1, 2, \dots & \text{if } j = \ell + 1/2 \end{cases}$$
(20.326)

We can then combine the 4 equations for f and g into 2 equations as

$$\frac{1}{\hbar c} \left[E + \frac{Ze^2}{r} + mc^2 \right] f - \left(\frac{dg}{dr} + (1+k)\frac{g}{r} \right) = 0$$
 (20.327)

$$\frac{1}{\hbar c} \left[E + \frac{Ze^2}{r} - mc^2 \right] g + \left(\frac{df}{dr} + (1-k)\frac{f}{r} \right) = 0$$
(20.328)

Setting

$$\begin{split} F &= rf \quad , \quad G = rg \\ \alpha_1 &= \frac{mc^2 + E}{\hbar c} \quad , \quad \alpha_2 = \frac{mc^2 - E}{\hbar c} \\ \alpha &= (\alpha_1 \alpha_2)^{1/2} \quad , \quad \gamma = \frac{Ze^2}{\hbar c} \quad , \quad \rho = \alpha r \end{split}$$

we get

$$\begin{pmatrix} \frac{d}{d\rho} + \frac{k}{\rho} \end{pmatrix} G - \left(\frac{\alpha_1}{\alpha} + \frac{\gamma}{\rho} \right) F = 0$$

$$\begin{pmatrix} d & k \end{pmatrix} F = \begin{pmatrix} \alpha_2 & \gamma \\ \alpha_2 & \gamma \end{pmatrix} G = 0$$

$$(20.329)$$

$$\left(\frac{d}{d\rho} - \frac{\kappa}{\rho}\right)F - \left(\frac{\alpha_2}{\alpha} - \frac{\gamma}{\rho}\right)G = 0$$
(20.330)

We now solve these coupled equations using the standard series method to obtain the positive energy bound state solutions.

We substitute

$$F = \phi(\rho)e^{-\rho}$$
, $F = \chi(\rho)e^{-\rho}$ (20.331)

and obtain

$$\chi' - \chi + \frac{k}{\rho}\chi - \left(\frac{\alpha_1}{\alpha} + \frac{\gamma}{\rho}\right)\phi = 0$$
(20.332)

$$\phi' - \phi - \frac{k}{\rho}\phi - \left(\frac{\alpha_2}{\alpha} - \frac{\gamma}{\rho}\right)\chi = 0$$
(20.333)

We now substitute the series

$$\phi = \rho^s \sum_{m=0}^{\infty} a_m \rho^m \quad , \ a_0 \neq 0 \quad , \quad \chi = \rho^s \sum_{m=0}^{\infty} b_m \rho^m \quad , \ b_0 \neq 0 \tag{20.334}$$

the requirement that f and g be finite everywhere turns out to be impossible to satisfy. Instead, we require that the integrated probability density be finite, i.e.,

$$\int_{0}^{\infty} \left[|F(\rho)|^{2} + |G(\rho)|^{2} \right] d\rho < \infty$$
(20.335)
This makes sure that $s \neq -\infty$. Substituting the series and equating coefficients of the same power of ρ we get the recursion relations

$$(s+\nu+k)b_{\nu} - b_{\nu-1} - \gamma a_{\nu} - \frac{\alpha_1}{\alpha}a_{\nu-1} = 0$$
(20.336)

$$(s+\nu-k)a_{\nu} - a_{\nu-1} + \gamma b_{\nu} - \frac{\alpha_2}{\alpha}b_{\nu-1} = 0$$
(20.337)

For $\nu = 0$ we get

$$(s+k)b_0 - \gamma a_0 = 0 = (s-k)a_0 + \gamma b_0 \tag{20.338}$$

These equations have a nontrivial solution if and only if

$$s = \pm (k^2 - \gamma^2)^{1/2} \tag{20.339}$$

First we look at the negative root. For small ρ the integrand for the integrated probability density is ~ ρ^{2s} and we must have 2s > -1 or $(k^2 - \gamma^2)^{1/2} > 1/2$. The minimum s occurs when $k^2 = 1$. This corresponds to $Z \ge 109$. For $k^2 > 1$, no value of Z will permit the negative root.

Restricting ourselves to Z < 109, we choose the positive root $s = (k^2 - \gamma^2)^{1/2}$. For k = 1, s < 1, f and g diverge at the origin. The probability density integral converges, however.

The recursion relations lead to function of the order $e^{2\rho}$ (the probability density integral would diverge) unless the series terminate. Suppose the series terminate for $\nu = n'$, i.e., $a_{n'+1} = b_{n'+1} = 0$. We then have from the recursion relations that

$$\alpha_1 a_{n'} = -\alpha b_{n'} \quad , \quad n' = 0, 1, 2, \dots$$
 (20.340)

We now multiply the first recursion relation by α and the second by α_1 and subtract them to get

$$b_{\nu}[\alpha(s+\nu+k)-\alpha_{1}\gamma] = a_{\nu}[\alpha_{1}(s+\nu-k)+\alpha\gamma]$$
(20.341)

Inserting $\nu = n'$ and using $\alpha_1 a_{n'} = -\alpha b_{n'}$ we get

$$2\alpha(s+n') = \gamma(\alpha_1 - \alpha_2) = \frac{2E\gamma}{\hbar c}$$
(20.342)

Putting everything together we get

$$E = mc^{2} \left[1 + \frac{\gamma^{2}}{(s+n')^{2}} \right]^{-1/2} = mc^{2} \left[1 + \frac{\gamma^{2}}{\left(n' + \sqrt{k^{2} - \gamma^{2}}\right)^{2}} \right]^{-1/2}$$
(20.343)

Since $|k| = j + \frac{1}{2}$ we get

$$E = mc^{2} \left[1 + \frac{\gamma^{2}}{\left(n' + \sqrt{\left(j + \frac{1}{2}\right)^{2} - \gamma^{2}} \right)^{2}} \right]^{-1/2}, n' = 0, 1, 2... \quad j + \frac{1}{2} = 1, 2, 3, ...$$
(20.344)

where $\gamma = Ze^2/\hbar c$.

Before looking at the physics in this result let us investigate an alternative approach involving a second-order Dirac Equation. The first-order Dirac equation is

$$\beta \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \psi(\vec{r}, t) = 0 \quad , \quad \hat{H} = c\vec{\alpha} \cdot \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right) + \beta mc^2 + e\Phi \qquad (20.345)$$

We now define the projection operator \hat{P} as

$$\hat{P} = \frac{\beta \left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right) + 2mc^2}{2mc^2}$$
(20.346)

and operate on the Dirac equation from the left. After some algebra we get

$$\left[\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)^2 - \left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)^2 - m^2c^2 + \frac{e\hbar}{c}\left(\vec{\sigma}\cdot\vec{B} - i\vec{\alpha}\cdot\vec{\varepsilon}\right)\right]\psi = 0 \quad (20.347)$$

where we have used the relations

$$\left[\vec{\alpha} \cdot \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}\right)\right]^2 = \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}\right)^2 - \frac{e\hbar}{c} \vec{\sigma} \cdot \vec{B}$$
(20.348)

and

$$\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}, i\hbar\frac{\partial}{\partial t} - e\Phi\right] = -i\hbar e\vec{\varepsilon}$$
(20.349)

The new second-order equation is just the Klein-Gordon equation with an additional term $(\vec{\sigma} \cdot \vec{B} - i\vec{\alpha} \cdot \vec{\varepsilon})$, which represents the direct coupling of the electromagnetic fields to the magnetic (and electric) moments of the particle.

Every solution of the Dirac equation is a solution of this new second-order equation, but every solution of the second-order equation in not necessarily a solution of the Dirac equation.

If, however, ψ is a solution of the second-order equation, then $\phi = \hat{P}\psi$ is a solution of the Dirac equation. We can see this as follows. The second-order equation can be written as

$$\hat{P}\beta\left(i\hbar\frac{\partial}{\partial t}-\hat{H}\right)\psi(\vec{r},t) = \beta\left(i\hbar\frac{\partial}{\partial t}-\hat{H}\right)\hat{P}\psi(\vec{r},t) = 0$$
(20.350)

or the second order equation is equivalent to

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\psi(\vec{r}, t) = \left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\phi(\vec{r}, t) = 0$$
(20.351)

This says that \hat{P} acts as a projection operator, which reduces solutions of the second-order equation to solutions of the first-order Dirac equation.

Let us now use the second-order equation to find the energy levels of the Dirac hydrogen atom (Glauber, et al PR 109,1307(1958)). For a stationary state of energy E in the Coulomb potential the second-order equation becomes

$$\left[\frac{1}{c^2}\left(E + \frac{Ze^2}{r}\right)^2 - \left(\frac{\hbar}{i}\nabla\right)^2 - m^2c^2 + \frac{i\hbar Ze^2}{r^2c}\alpha_r\right]\psi = 0$$
(20.352)

where $\alpha_r = \vec{\alpha} \cdot \hat{r}$. We now write

$$\left(\frac{\hbar}{i}\nabla\right)^2 = -\frac{\hbar^2}{r^2}\frac{\partial^2}{\partial r^2}r^2 + \frac{\hat{L}^2}{r^2}$$
(20.353)

and get the equation

$$\left[\frac{E^2 - m^2 c^4}{c^2} + \frac{2EZe^2}{rc^2} + \frac{\hbar^2}{r^2} \frac{\partial^2}{\partial r^2} r^2 - \frac{\hat{L}^2 - \left(\frac{Ze^2}{c}\right)^2 - i\hbar\left(\frac{Ze^2}{c}\right)\alpha_r}{r^2}\right]\psi = 0 \quad (20.354)$$

We now use a few tricks to change this equation, which is almost in the same form as the Klein-Gordon equation for the Coulomb potential, into exactly the same form.

We first define the operator

$$\hat{K} = \beta \left(1 + \vec{\sigma} \cdot \frac{\vec{L}}{\hbar} \right) \tag{20.355}$$

with these properties

$$[\hat{K}, \vec{\alpha} \cdot \vec{p}] = 0$$
 , $[\hat{K}, \vec{\alpha} \cdot \vec{r}] = 0$, $[\hat{K}, r^2] = 0$ (20.356)

$$\begin{bmatrix} \hat{K}, \vec{J} \end{bmatrix} = 0 \quad , \quad \vec{J} = \vec{L} + \frac{\hbar}{2}\vec{\sigma}$$
 (20.357)

These imply that \hat{K} commutes with the Hamiltonian

$$\hat{H} = c\vec{\alpha} \cdot \vec{p} + \beta mc^2 - \frac{Ze^2}{r}$$
(20.358)

for the relativistic hydrogen atom.

This says that \hat{K} is a constant of the motion and since it also commutes with the total angular momentum we can label the common eigenstates or energy levels of the hydrogen atom by the eigenvalues of \hat{K} , \hat{J}^2 and \hat{J}_z . \hat{K} is a constant of the motion for any spherically symmetric, spin-independent potential and physically it measures the degree to which the spin and the orbital angular momentum of the particle are aligned.

Let us find the eigenvalues k of \hat{K} . We note that

$$\hat{K}^{2} = \left(1 + \vec{\sigma} \cdot \frac{\vec{L}}{\hbar}\right)^{2} = 1 + \left(\vec{\sigma} \cdot \frac{\vec{L}}{\hbar}\right)^{2} + 2\vec{\sigma} \cdot \frac{\vec{L}}{\hbar}$$

$$= 1 + \left(\frac{\vec{L} \cdot \vec{L}}{\hbar^{2}} + \frac{i}{\hbar^{2}}\vec{\sigma} \cdot (\vec{L} \times \vec{L})\right) + 2\vec{\sigma} \cdot \frac{\vec{L}}{\hbar}$$

$$= 1 + \left(\frac{\vec{L} \cdot \vec{L}}{\hbar^{2}} + \frac{i}{\hbar^{2}}\vec{\sigma} \cdot (i\hbar\vec{L})\right) + 2\vec{\sigma} \cdot \frac{\vec{L}}{\hbar}$$

$$= 1 + \frac{L^{2}}{\hbar^{2}} + \vec{\sigma} \cdot \frac{\vec{L}}{\hbar} = \frac{1}{\hbar^{2}} \left(\vec{L} + \frac{\hbar}{2}\vec{\sigma}\right)^{2} + \frac{1}{4}$$

$$= \frac{\hat{J}^{2}}{\hbar^{2}} + \frac{1}{4}$$
(20.359)

where we have used

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + i\vec{\sigma} \cdot (\vec{A} \times \vec{B})$$
$$\vec{L} \times \vec{L} = i\hbar \vec{L} \quad , \quad \vec{J} = \vec{L} + \vec{S} \quad , \quad \vec{S} = \frac{\hbar}{2}\vec{\sigma}$$

Therefore, we have

$$k^{2} = j(j+1) + \frac{1}{4} = (j+\frac{1}{2})^{2}$$
(20.360)

Now, since $\left\{ \hat{K},\gamma_{5}\right\} =0$ we find that, if k is an eigenvalue of $\hat{K},$ i.e.,

$$\hat{K}|k\rangle = k|k\rangle \tag{20.361}$$

then

$$\hat{K}\gamma_5 |k\rangle = -\gamma_5 \hat{K} |k\rangle = -k\gamma_5 |k\rangle \qquad (20.362)$$

which says that -k is also an eigenvalue of \hat{K} . The eigenvalues are then

$$k = \pm 1, \pm 2, \pm 3, \dots$$
 (20.363)

since $j = 1/2, 3/2, 5/2, \ldots$ Note that zero is not an eigenvalue of \hat{K} . In addition, an eigenstate of \hat{K} with eigenvalue k is an eigenstate of \hat{J}^2 with eigenvalue j = |k| - 1/2.

We now find the energy eigenvalues. Define the operator

$$\hat{\Lambda} = -\beta \hat{K} - i \frac{Ze^2}{\hbar c} \alpha_r \tag{20.364}$$

with the properties

$$\left[\hat{\Lambda}, \hat{K}\right] = 0 \quad , \quad \left[\hat{\Lambda}, \vec{J}\right] = 0 \quad , \quad \Lambda^2 = K^2 - \left(\frac{Ze^2}{\hbar c}\right)^2 \tag{20.365}$$

A little algebra then shows that

$$\hbar^2 \hat{\Lambda} (\hat{\Lambda} + 1) = \hat{L}^2 - \left(\frac{Ze^2}{c}\right)^2 - i\hbar \left(\frac{Ze^2}{c}\right) \alpha_r \qquad (20.366)$$

which is the operator in the last term of the second-order equation. We can then write

$$\left[\frac{E^2 - m^2 c^4}{c^2} + \frac{2EZe^2}{rc^2} + \frac{\hbar^2}{r^2}\frac{\partial^2}{\partial r^2}r^2 - \frac{\hbar^2\hat{\Lambda}(\hat{\Lambda}+1)}{r^2}\right]\psi = 0$$
(20.367)

This is exactly the same form as the Klein-Gordon equation except that

$$\ell'(\ell'+1) \to \hat{\Lambda}(\hat{\Lambda}+1) \tag{20.368}$$

or a number has been replaced by an operator. Now if $\psi(\vec{r})$ is an eigenstate of $\hat{\Lambda}(\hat{\Lambda}+1)$ then the operator $\hat{\Lambda}(\hat{\Lambda}+1)$ in the equation is replaced by its eigenvalue which we can write as $\ell'(\ell'+1)$. This says that the energy eigenvalues are given by the same formula as in the spin zero case, i.e.,

$$E = \frac{mc^2}{\left[1 + \left(\frac{Ze^2}{\hbar cn'}\right)^2\right]^{1/2}} \quad , \quad n' = \ell' + 1 + \nu \quad , \quad \nu = 0, 1, 2, \dots$$
(20.369)

Since $\hat{\Lambda}$, \hat{K} , \hat{J}^2 and \hat{J}_z all commute, we can construct solutions which are eigenstates of \hat{K} , \hat{J}^2 and \hat{J}_z as well as $\hat{\Lambda}$.

 $\hat{\Lambda}$ does not commute with \hat{H} however. This means that the solutions we have found for the second order equation cannot directly be eigenfunctions of \hat{H} . Instead, since

$$\hat{H}(\hat{P}\psi) = E(\hat{P}\psi) \tag{20.370}$$

i.e., the energy eigenvalues from the second-order equation are also the eigenvalues of \hat{H} , we can find eigenfunctions of \hat{H} by using the projection operator \hat{P} . Since \hat{P} and $\hat{\Lambda}$ do not commute, the eigenfunction of \hat{H} , namely $\hat{P}\psi$, will generally be a linear combination of different $\hat{\Lambda}$ eigenfunctions.

To find the energy eigenvalues we need to know the eigenvalues of $\hat{\Lambda}$. Consider an eigenstate of $\hat{\Lambda}$ and \hat{K} with eigenvalues k. We then have

$$\hat{\Lambda}^2 |k\rangle = \lambda^2 |k\rangle = \left(\hat{K}^2 - \left(\frac{Ze^2}{\hbar c}\right)^2\right)|k\rangle = \left(k^2 - \left(\frac{Ze^2}{\hbar c}\right)^2\right)|k\rangle \tag{20.371}$$

or

$$\lambda = \left(k^2 - \left(\frac{Ze^2}{\hbar c}\right)^2\right)^{1/2} \tag{20.372}$$

and the possible eigenvalues of $\hat{\Lambda}$ are $\pm \lambda$. When $\hat{\Lambda}(\hat{\Lambda} + 1)$ acts on a $(\hat{\Lambda}, \hat{K})$ eigenstate it has the eigenvalue $\pm \lambda(\pm \lambda + 1) = \ell'(\ell' + 1)$. This leads to two possible ℓ' values for each eigenvalue of $\hat{\Lambda}$:

$$\ell' = \begin{cases} \lambda, -\lambda - 1 & \text{for } \Lambda = \lambda \\ -\lambda, \, \lambda - 1 & \text{for } \Lambda = -\lambda \end{cases}$$
(20.373)

For each eigenvalue of $\hat{\Lambda}$, the two ℓ' solutions add up to -1. The smaller of the two solutions -lambda and $-\lambda - 1$ are eliminated because they are not normalizable (behavior near the origin). This leave two cases to consider:

(1)
$$\Lambda = \lambda$$
 , $\ell' = \lambda$
(2) $\Lambda = -\lambda$, $\ell' = \lambda - 1$

The possible energy eigenvalues are given by

$$E = \frac{mc^2}{\left[1 + \left(\frac{Ze^2}{\hbar cn'}\right)^2\right]^{1/2}} \quad , \quad n' = \ell' + 1 + \nu \quad , \quad \nu = 0, 1, 2, \dots$$
(20.374)

or redefining some quantities

$$n' = n - |k| + \lambda = n - j - \frac{1}{2} + \sqrt{\left(j + \frac{1}{2}\right)^2 - \left(\frac{Ze^2}{\hbar c}\right)^2}$$
(20.375)

so that n takes on the values

$$n = |k| , |k| + 1 , |k| + 2 , \dots \text{for} \Lambda = -\lambda$$

$$n = |k| + 1 , |k| + 2 , |k| + 3 , \dots \text{for} \Lambda = \lambda$$

the energy levels are then given by

$$E = mc^{2} \left[1 + \frac{\left(\frac{Ze^{2}}{\hbar c}\right)^{2}}{\left[n - j - \frac{1}{2} - \sqrt{\left(j + \frac{1}{2}\right)^{2} - \left(\frac{Ze^{2}}{\hbar c}\right)^{2}}\right]^{2}} \right]^{-1/2}$$
(20.376)

The quantum number n is just the principal quantum number of the hydrogen atom.

The energy level structure looks like Figure 20.2 below.

| | n = k + 2 | n = k + 2 |
|----|-------------|-------------|
| Е↑ | n = k + 1 | n = k + 1 |
| | n = k | |

Figure 20.2: Dirac hydrogen energy level structure

where the left sequence corresponds to $\Lambda = -\lambda$ and the right sequence to $\Lambda = \lambda$.

Some Features

The energy levels for the spin 1/2 particle are the same as those found for the spin 0 particle with $\ell \rightarrow j$.

The energy is real only if

$$j + \frac{1}{2} < \frac{Ze^2}{\hbar c}$$
(20.377)

which corresponds to Z < 137 for j = 1/2.

The Dirac theory leads to an accidental degeneracy in ℓ , i.e., states with the same j but different ℓ have the same energy. This degeneracy is removed by the Lamb shift, which is due to the interaction of the electron with its own field. As we shall see later, for j = 1/2, the effect is one order of magnitude smaller then the fine structure splitting. For $j \ge 3/2$, it is two orders of magnitude smaller.

An expansion in powers of $Z\alpha$, where

$$\alpha = \frac{e^2}{\hbar c} = \text{ fine structure constant}$$
(20.378)

looks like

$$E_{n,j} = mc^2 \left[1 - \frac{Z^2 \alpha^2}{2n^2} - \frac{(Z\alpha)^4}{2n^3} \left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right) + O((Z\alpha)^6) \right]$$
(20.379)

which agrees with the perturbation calculations we carried out earlier.

Some Details about the Energy Levels

The solutions of the Dirac equation are not $\hat{\Lambda}$ eigenstates but they are \hat{K} eigenstates and \hat{K} is a constant of the motion (it commutes with the Hamiltonian). The total orbital angular momentum \vec{L} is not a constant of the motion and neither is \hat{L}^2 . We need to come up with some way to classify the energy levels in the relativistic hydrogen atom using the eigenvalues k.

To get a handle on how to proceed we look at the nonrelativistic limit where

$$\hat{\Lambda} \to -\beta \hat{K} \to -\hat{K}$$
 for positive energy states (20.380)

We expect the solutions of the second order equation with one sign of $\hat{\Lambda}$ to correspond to solutions of the first-order equation with the opposite sign of \hat{K} . This means that

$$\begin{split} n &= |k| \ , \ |k| + 1 \ , \ |k| + 2 \ , \ \dots \dots \text{ for } \Lambda = -\lambda \to k > 0 \\ n &= |k| + 1 \ , \ |k| + 2 \ , \ |k| + 3 \ , \ \dots \dots \text{ for } \Lambda = \lambda \to k < 0 \end{split}$$

It turns out to be convenient to still label the solutions by the ℓ value that they would have in the nonrelativistic limit. To find this ℓ value we use

$$\hat{K}^2 = 1 + \frac{\hat{L}^2}{\hbar^2} + \vec{\sigma} \cdot \frac{\vec{L}}{\hbar} = \beta \hat{K} + \frac{\hat{L}^2}{\hbar^2}$$
$$\hat{K}(\hat{K} - \beta) = \frac{\hat{L}^2}{\hbar^2}$$

In the nonrelativistic limit, $\beta \rightarrow 1$ and we have

$$\hat{K}(\hat{K}-1) = \frac{\hat{L}^2}{\hbar^2} \to k(k-1) = \ell(\ell+1)$$
(20.381)

so that ℓ becomes the total orbital angular momentum quantum number in the nonrelativistic limit. Solving for ℓ in terms of k we get

$$\ell = \begin{cases} k - 1 = j - 1/2 & \text{for } k > 0\\ |k| = j + 1/2 & \text{for } k < 0 \end{cases}$$
(20.382)

Now K measures the alignment of the spin and the orbital angular momentum. The above results say that for k > 0, they are essentially parallel and so $j = \ell + 1/2$ and for k < 0 they are essentially antiparallel so $j = \ell - 1/2$.

A detailed calculation of the wave functions shows that the upper two components of the wave function (the large components) are eigenstates of total orbital angular momentum with eigenvalue ℓ , while the lower two components (the small components) are eigenstates of total orbital angular momentum with eigenvalue $\ell + 1$ for k > 0 and with $\ell - 1$ for k < 0.

The complete energy level scheme for the relativistic hydrogen atom for n = 1, 2, and 3 looks like Figure 20.3 below.



Figure 20.3: Energy level structure for relativistic hydrogen

The complete degeneracy of a given n in the nonrelativistic case is lifted by relativistic effects. The degeneracy between states like $1S_{1/2}$, $2P_{3/2}$, $3D_{5/2}$, $4F_{7/2}$, etc is now broken. The degeneracy still remains between states like $2S_{1/2}$ and $2P_{1/2}$, $3S_{1/2}$ and $3P_{1/2}$, $3P_{3/2}$ and $3D_{3/2}$, etc., levels.

All levels except $1S_{1/2}$, $2P_{3/2}$, $3D_{5/2}$, etc., are 2-fold degenerate because they are the eigenstates of of K with opposite eigenvalues, i.e., $2P_{3/2} \rightarrow k = 2$, $2D_{3/2} \rightarrow k = -2$.

Hyperfine Structure

The are two corrections that modify the energy level results from the Dirac equation. The two-fold degeneracy is removed by the interaction of the electron with vacuum fluctuations of the electromagnetic radiation field. This effect is called the Lamb shift. In addition, there is also a hyperfine interaction which splits every level into two, It is due to the interaction of the electron with the magnetic moment of the proton. We consider hyperfine splitting first.

As an example we derive the hyperfine splitting of an s-state using nonrelativistic first-order perturbation theory. The interaction of the electron spin with the magnetic moment of the proton is given by

$$\hat{H}' = \frac{|e|h}{2mc}\vec{\sigma}\cdot\vec{B}(\vec{r}) = \mu_B\vec{\sigma}\cdot\vec{B}(\vec{r})$$
(20.383)

where $\vec{B}(\vec{r})$ is the magnetic field due to the magnetic moment of the proton. This magnetic moment is given by

$$\vec{M}_{p} = \frac{|e| \hbar g_{p}}{4m_{p}c} \vec{\sigma}_{p} = \frac{1}{2} g_{p} \mu_{p} \vec{\sigma}_{p}$$
(20.384)

where g_p is the gyromagnetic ratio of the proton, m_p is the proton mass and $\hbar \vec{\sigma}_p/2$ is the spin of the proton. The magnetic field from this magnetic moment

(assuming the proton is fixed at the origin) is given by the relations

$$\vec{A}(\vec{r}) = -\vec{M}_p \times \nabla\left(\frac{1}{r}\right) = \text{vector potential}$$
 (20.385)

$$\vec{B}(\vec{r}) = \nabla \times \vec{A}(\vec{r}) \tag{20.386}$$

$$\vec{B}(\vec{r}) = -\nabla \times (\vec{\sigma}_p \times \nabla) \frac{g_p \mu_p}{2r}$$
(20.387)

This gives

$$\hat{H}' = -g_p \mu_B \mu_p \vec{\sigma} \cdot \left(\nabla \times (\vec{\sigma}_p \times \nabla) \frac{1}{2r} \right)$$

$$= -g_p \mu_B \mu_p \vec{\sigma} \cdot (\vec{\sigma}_p (\nabla \cdot \nabla) - \nabla (\vec{\sigma}_p \cdot \nabla)) \frac{1}{2r}$$

$$= -g_p \mu_B \mu_p \left((\vec{\sigma} \cdot \vec{\sigma}_p) (\nabla \cdot \nabla) - (\vec{\sigma} \cdot \nabla) (\vec{\sigma}_p \cdot \nabla) \right) \frac{1}{2r}$$
(20.388)

The first-order shift of the level is

$$\left\langle \hat{H}' \right\rangle = -g_p \mu_B \mu_p \int d^3 r \left| \psi(\vec{r}) \right|^2 \left[\left(\left\langle \vec{\sigma} \cdot \vec{\sigma}_p \right\rangle (\nabla \cdot \nabla) - \left\langle \left(\vec{\sigma} \cdot \nabla \right) (\vec{\sigma}_p \cdot \nabla) \right\rangle \right) \frac{1}{2r} \right]$$
(20.389)

where the brackets $\langle \dots \rangle$ denote the expectation value in the relative spin state of the electron and proton and $\psi(\vec{r})$ is the nonrelativistic wave function of the level. If we only consider *s*-states, which are spherically symmetric, then

$$\langle (\vec{\sigma} \cdot \nabla) (\vec{\sigma}_p \cdot \nabla) \rangle = \frac{1}{3} \langle (\vec{\sigma} \cdot \vec{\sigma}_p) \rangle \nabla^2$$
(20.390)

and we get

where we have used

$$\nabla^2 \frac{1}{r} = -4\pi\delta(\vec{r}) \tag{20.392}$$

For the hydrogen atom s-state

$$\left|\psi(0)\right|^2 = \frac{1}{\pi (na_0)^3} \tag{20.393}$$

and we get

$$\left\langle \hat{H}' \right\rangle = \frac{2}{3} \left(\frac{e^2}{2a_0} \right) g_p \frac{m}{m_p} \frac{\alpha^2}{n^3} \left\langle \left(\vec{\sigma} \cdot \vec{\sigma}_p \right) \right\rangle \tag{20.394}$$

We then have

$$\vec{F} = \vec{S} + \vec{I} = \text{ total spin} \tag{20.395}$$

For $S = \frac{1}{2}$, $I = \frac{1}{2}$, we have F = 0(singlet), 1(triplet). But

$$\vec{F} = \vec{S} + \vec{I} \to \vec{F}^2 = \vec{S}^2 + \vec{I}^2 + 2\vec{S} \cdot \vec{I}$$
 (20.396)

$$\vec{S} \cdot \vec{I} = \frac{\hbar^2}{4} \vec{\sigma} \cdot \vec{\sigma}_p = \frac{\hbar^2}{2} (F(F+1) - 3/2)$$
(20.397)

We then have for a relative triplet state $\langle (\vec{\sigma} \cdot \vec{\sigma}_p) \rangle = 1$ and for a relative singlet state $\langle (\vec{\sigma} \cdot \vec{\sigma}_p) \rangle = -3$. This says that the singlet state lies lower than the triplet.

The total splitting of the ground state is

$$\Delta E = \frac{8}{3} \left(\frac{e^2}{2a_0} \right) g_p \frac{m}{m_p} \alpha^2 \tag{20.398}$$

between the triplet and singlet. The transition between these two levels generates radiation with a frequency of 1420 MHz and a wavelength of 21.4 cm. This radiation is very important in astronomy. From its intensity, Doppler broadening, and Doppler shift, one obtains information concerning the density, temperature, and motion of interstellar and intergalactic hydrogen clouds.

The Lamb Shift

The coupling

$$\hat{H}_{\rm int} = -\frac{e}{c} \int d^3 \vec{rj}(\vec{r}) \cdot \vec{A}(\vec{r})$$
(20.399)

of the electron to the quantum mechanical radiation field causes a shift in the energy levels of the hydrogen atom. Although not an exact calculation, we can get some idea of the fundamental difficulties in quantum electrodynamics by doing a nonrelativistic second-order perturbation calculation.

We consider an electron in the state $|n\rangle$ with energy ε_n . Because of the above interaction (see last part of this chapter) the electron is able to spontaneously emit a photon thereby going to some state $|n'\rangle$. This produces a second-order shift in the energy given by

$$\Delta E_n = \sum_{n'} \sum_{\vec{k}\vec{\lambda}} \frac{\left| \left\langle n', \vec{k}\vec{\lambda} \right| \hat{H}_{\text{int}} \left| n, 0 \right\rangle \right|^2}{\varepsilon_n - \varepsilon_{n'} - ck}$$
(20.400)

where $|n, 0\rangle$ is the initial state with the electron in $|n\rangle$ with no photons present, and $|n', \vec{k}\vec{\lambda}\rangle$ is the intermediate state with an electron in $|n'\rangle$ and on photon of momentum \vec{k} and polarization $\vec{\lambda}$ present. The energy of this intermediate state is $\varepsilon_{n'} + ck$. From the quantum theory of electromagnetic radiation (see end of this chapter) we have that

$$\left\langle n', \vec{k}\vec{\lambda} \right| \hat{H}_{\text{int}} \left| n, 0 \right\rangle = -\frac{e}{c} \sqrt{\frac{2\pi\hbar^2 c^2}{\omega_k V}} \left\langle n' \right| \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \left| n \right\rangle \tag{20.401}$$

where $\vec{j}_{\vec{k}}$ is the k^{th} Fourier component of the current $\vec{j}(\vec{r})$. Therefore,

$$\Delta E_n = \int \frac{d^3k}{(2\pi\hbar)^3} \frac{2\pi\hbar^2 e^2}{ck} \sum_{n'} \frac{\sum_{\lambda} \left| \langle n' | \, \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \, |n \rangle \right|^2}{\varepsilon_n - \varepsilon_{n'} - ck}$$
$$= \int \frac{k^2 dk}{4\pi^2 \hbar} \frac{e^2}{ck} \sum_{n'} \frac{\int d\Omega \sum_{\lambda} \left| \langle n' | \, \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \, |n \rangle \right|^2}{\varepsilon_n - \varepsilon_{n'} - ck}$$
(20.402)

In the dipole approximation, we can use

$$\vec{j}_{\vec{k}} \to \vec{j}_0 = \frac{\vec{p}}{m} \quad , \quad \vec{p} = \text{ electron momentum operator}$$
(20.403)

The angular integration over the polarizations is given by

$$\int d\Omega \sum_{\vec{\lambda}} \left| \langle n' | \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* | n \rangle \right|^2 = \frac{1}{m} \int d\Omega \sum_{\vec{\lambda}} \left| \langle n' | \vec{p} \cdot \vec{\lambda}^* | n \rangle \right|^2 = \frac{4\pi}{m} \frac{2}{3} \left| \langle n' | \vec{p} | n \rangle \right|^2$$

where the factor 2/3 comes from the fact that there are only 2 independent polarizations for each \vec{k} value. This gives

$$\Delta E_n = \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty \omega d\omega \sum_{n'} \frac{|\langle n'|\vec{p}\,|n\rangle|^2}{\varepsilon_n - \varepsilon_{n'} - \omega} \quad , \quad \omega = ck \tag{20.404}$$

The first problem we encounter is that the ω integral diverges!! This means that the interaction with the radiation field produces an *infinite shift downward* in the energy of the electron.

This result presented theoretical physics with a great difficulty for many years. In the late 1940's it was resolved due to the work of Feynman, Schwinger and Tomonaga in producing new calculation rules within the context of quantum electrodynamics and by Bethe and Weisskopf who actually carried out the calculation using the new rules and got a finite number agreeing with experiment.

Let us try to understand some aspects of what happened.

If we do a similar calculation for a free electron, then one gets an infinite result again. In the dipole approximation, we can evaluate the energy shift for a free electron in a momentum state $|\vec{p}\rangle$. We get

$$\Delta E_{\vec{p}} = \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty \omega d\omega \sum_{\vec{q}} \frac{|\langle \vec{q} | \vec{p} | \vec{p} \rangle|^2}{\varepsilon_q - \varepsilon_p - \omega}$$
(20.405)

Since this is a free particle $\varepsilon_q - \varepsilon_p = 0$ and we have

$$\Delta E_{\vec{p}} = -\frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty \omega d\omega \frac{\left|\langle \vec{p} | \vec{p} | \vec{p} \rangle\right|^2}{\omega} = -\frac{2e^2}{3\pi\hbar c^3 m^2} p^2 \int_0^\infty d\omega \qquad (20.406)$$

which is infinite. What Bethe and Weisskopf noticed was that this expression is proportional to p^2 . In their development of quantum electrodynamics, Feynman, Schwinger and Tomonaga had similar problems which they were able to deal with be redefining the electron parameters that appeared in the theory (like mass and charge). The process is called *renormalization*. In this process all infinite expression are consistently incorporated into the mass or charge parameters and then these are defined to have the known experimental values.

In our case, we can interpret the infinite result as redefining the mass, i.e., as representing a shift of the mass of the electron. In terms of the mathematics, this means the following. If we say that m_0 is the mass and $p^2/2m_0$ is the kinetic energy of a free electron of momentum \vec{p} neglecting the electromagnetic interactions, then the energy including the effects of the electromagnetic interactions is given by

$$\frac{p^2}{2m_0} + \Delta E_{\vec{p}} = \left(\frac{1}{m_0} - \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty d\omega\right) \frac{p^2}{2} = \frac{1}{m} \frac{p^2}{2}$$
(20.407)

i.e., we have *renormalized* the electron mass. The so-called electromagnetic selfenergy of the electron can thus be interpreted as giving a shift of the mass of the electron from its *bare* (no electromagnetic interactions) value m_0 to its *observed* (measured in the laboratory where all interactions are present) value m.

We then argue that the reason the interacting electron has an infinite energy shift is that it includes the infinite energy change that we already have counted once when we use the observed mass m rather than the bare mass in the calculation and, thus, we are double counting. In other words, we should really start out with the Hamiltonian for the hydrogen atom in the presence of the radiation field given by

$$\hat{H} = \frac{p^2}{2m_0} - \frac{e^2}{r} + \hat{H}_{\rm int}$$
(20.408)

Then using the corrected expression for m we get

$$\hat{H} = \frac{p^2}{2m} - \frac{e^2}{r} + \left(\hat{H}_{\text{int}} + \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty d\omega\right)$$
(20.409)

This means that if we write the observed free particle mass in the kinetic energy (which we always do) we should not count that part of \hat{H}_{int} that produces the infinite mass shift, i.e., we should regard

$$\hat{H}_{\rm int} + \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty d\omega$$
 (20.410)

as the effective interaction of an electron of renormalized mass m with the radiation field. It is now finite to second-order of our calculation. Feynman, et al, showed that this could be done to all orders of perturbation theory!!

We therefore modify our calculation by adding in the required term. We get

$$\Delta E'_{n} = \frac{2e^{2}}{3\pi\hbar c^{3}m^{2}} \int_{0}^{\infty} \omega d\omega \left(\sum_{n'} \frac{\left| \langle n' | \vec{p} | n \rangle \right|^{2}}{\varepsilon_{n} - \varepsilon_{n'} - \omega} + \frac{\left| \langle n | \vec{p} | n \rangle \right|^{2}}{\omega} \right)$$
(20.411)

Using completeness, we have

$$\langle n | p^{2} | n \rangle = \sum_{n'} \langle n | p | n' \rangle \langle n' | p | n \rangle = \sum_{n'} |\langle n' | p | n \rangle|^{2}$$
 (20.412)

so that

$$\Delta E'_{n} = \frac{2e^{2}}{3\pi\hbar c^{3}m^{2}} \sum_{n'} \left| \langle n'|p|n \rangle \right|^{2} \int_{0}^{\infty} d\omega \frac{\varepsilon_{n'} - \varepsilon_{n}}{\varepsilon_{n} - \varepsilon_{n'} - \omega}$$
(20.413)

The integral is still divergent but only logarithmically and, in fact, not at all in more sophisticated relativistic calculations. We can imagine that the correct calculation would yield a similar result but with a convergent integral. We can simulate this result by integrating to some cutoff value (and not to infinity) say at $\hbar\omega = mc^2$. We then get

$$\Delta E'_{n} = \frac{2e^{2}}{3\pi\hbar c^{3}m^{2}} \sum_{n'} \left| \langle n' | p | n \rangle \right|^{2} (\varepsilon_{n'} - \varepsilon_{n}) \ell n \left| \frac{mc^{2}}{\varepsilon_{n'} - \varepsilon_{n}} \right|$$
(20.414)

where we have neglected quantities the size of $\varepsilon_{n'} - \varepsilon_n$ in comparison to mc^2 .

Be the evaluated this result numerically and obtained $\Delta E'_n = +1040$ megacycles (the $2P_{1/2}$ level turns out to be shifted downward) and the observed value equals +1057 megacycles, which is remarkable agreement!

Taking into account both the Lamb shift and the hyperfine splitting we have the level scheme shown in Figure 20.4 below for n = 2:



Figure 20.4: n = 2 Energy level structure for relativistic hydrogen

Dirac Hole Theory

Finally, we tackle the problem of the negative energy states in the Dirac theory.

As we said earlier, there is no simple conservation law that prevents an electron or any other spin 1/2 particle in a positive energy state from making a radiative transition to a negative energy state. This means all atoms must be unstable! An energy diagram is shown in Figure 20.5 below.



Figure 20.5: n = 2 Energy level structure for relativistic hydrogen

The properties of the positive energy states show remarkable agreement with

experiment. Can we simply ignore the negative energy states? The answer is no because an arbitrary wave packet, as we saw earlier will always contain negative energy components via interactions even if we start off only with positive energy components.

Dirac proposed a clever way out of this dilemma : since spin 1/2 particles obey the exclusion principle, all one needs to do to insure stability is to say that the negative energy states are completely filled. Then a particle cannot make a transition from a positive to a negative energy state for this would put two particles into the same (negative energy) state. The vacuum state in this picture consists of an *infinite sea* of particles in negative energy states. The particle and charge density at every point is infinite. This is not a problem for the physical theory since Dirac contended that we only measure deviations from the vacuum. In the absence of any potential, the charge density of the negative sea is uniform and Dirac argued that this charge density can produce no forces, since by isotropy, the forces have no special direction to point!

Now this theory has some very useful special property. Suppose that we remove a negative energy electron from the vacuum. What is left behind is a *hole* in the negative energy sea. Measured with respect to the vacuum, the hole would appear to have positive charge and positive energy, i.e., since it is the absence of negative charge and negative energy. Dirac interpreted it as a positron, which is the electron antiparticle.



Figure 20.6: A hole appears

Let me say that again.... an excited state of the vacuum arises as shown in the figure. A negative energy electron is excited into a positive energy state, leaving behind a hole with charge -(-e) = +e and the same mass as the electron, which is the antiparticle. It looks like a positive charge since if we apply an electric field the infinite sea of electron translates opposite to the field direction, which is unobservable since the sea is infinite. However, the hole seems to be traveling in the direction of the field like a positive charge!

In this way, antiparticles appear in the Dirac theory as unoccupied negative energy states, which is very different from the way they appear in the spin zero theory.

This Dirac hole theory gives a simple description for pair production. Suppose that a photon of energy $> 2mc^2$ traveling through the vacuum is absorbed by a negative energy electron and the negative energy electron gets excited to a positive energy state. What remains, as we have said, is a hole in the negative energy sea, i.e., a positive energy positron and a positive energy electron. This says that pair production is simply the excitation of a particle from a negative to a positive energy state.

Since we could exchange the roles of positrons and electrons in the entire Dirac theory, electrons would appear as holes in a positron sea. This forces us to conclude that negative energy seas cannot have any physical reality. The *hole theory* is simply a mathematical model that allows us to do the correct *book-keeping* within the framework of a single-particle Dirac theory.

With a filled negative energy sea, the Dirac theory would become a manyparticle theory in which we are unable to take into account the interactions between these particles. The Dirac theory gives valid results only when these interactions can be neglected. For example, in the hydrogen atom, the modification of the Coulomb potential by vacuum polarization accounts for about 2.5% of the Lamb shift.

If we second-quantized the Dirac theory, we can treat both particles and antiparticles on the same basis.

The full relativistic quantum field theory of the electrons and positrons and their interactions with photons was carried out by Feynman, et al in a theory which is beyond the scope of these volumes.

20.7 Electromagnetic Radiation and Matter

20.7.1 Interacting with the Classical Radiation Field

We assume *classical* EM radiation in the *transverse gauge*, where

$$\phi(\vec{r},t) = 0$$
 , $\nabla \cdot \vec{A}(\vec{r},t) = 0$ (20.415)

The electric and magnetic fields are given in terms of the vector potential (in this gauge) by

$$\vec{\varepsilon}(\vec{r},t) = -\frac{1}{c} \frac{\partial \vec{A}(\vec{r},t)}{\partial t} \quad , \quad \vec{B}(\vec{r},t) = \nabla \times \vec{A}(\vec{r},t)$$
(20.416)

The electromagnetic energy is given by

$$E = \int d^{3}\vec{r} \frac{\varepsilon^{2}(\vec{r},t) + B^{2}(\vec{r},t)}{8\pi}$$
(20.417)

and the rate and direction of energy transport is given by the Poynting vector

$$\vec{\wp}(\vec{r},t) = \frac{c}{4\pi}\vec{\varepsilon}(\vec{r},t) \times \vec{B}(\vec{r},t)$$
(20.418)

The radiation field generated by a classical current $\vec{j}(\vec{r},t)$ is given by

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\vec{A}(\vec{r},t) = -\frac{4\pi}{c}j_{\perp}(\vec{r},t)$$
(20.419)

where \perp means the transverse/divergence-free part.

We first consider the *monochromatic plane wave* solution of this equation. It takes the form

$$\vec{A}(\vec{r},t) = \alpha \vec{\lambda} e^{i\vec{k}\cdot\vec{r}-i\omega t} + \alpha^* \vec{\lambda}^* e^{-i\vec{k}\cdot\vec{r}+i\omega t}$$
(20.420)

where

$$\omega = ck$$

 $\vec{\lambda} = \text{polarization vector with } |\vec{\lambda}|^2 = 1$
 $\alpha = \text{amplitude} = \text{constant}$

To insure that $\nabla \cdot \vec{A}(\vec{r},t) = 0$ we require $\vec{\lambda} \cdot \vec{k} = 0$ which corresponds to transverse polarizations only.

The energy per unit volume in the electromagnetic wave is

$$\frac{\varepsilon^2 + B^2}{8\pi} = \frac{\omega^2}{2\pi c^2} \left[\left| \alpha \right|^2 - \operatorname{Re} \left(\alpha^2 \lambda^2 e^{2i\vec{k}\cdot\vec{r} - 2i\omega t} \right) \right]$$
(20.421)

The quantity $\operatorname{Re}(..)$ oscillates in time and averages to zero so that the average energy density is

$$\frac{E}{volume} = \frac{\omega^2}{2\pi c^2} \left|\alpha\right|^2 \tag{20.422}$$

In a similar way the time average of the Poynting vector is

$$\frac{\omega^2}{2\pi c} \left| \alpha \right|^2 \hat{k} \tag{20.423}$$

Any general wave solution is a *linear superposition* of these monochromatic wave solutions.

$$\vec{A}(\vec{r},t) = \sum_{\vec{k}\vec{\lambda}} \left[A_{\vec{k}\vec{\lambda}} \vec{\lambda} \frac{e^{i\vec{k}\cdot\vec{r}-i\omega t}}{\sqrt{V}} + A^*_{\vec{k}\vec{\lambda}} \vec{\lambda}^* \frac{e^{-i\vec{k}\cdot\vec{r}+i\omega t}}{\sqrt{V}} \right]$$
(20.424)

where the sum is over all allowed \vec{k} values and over the two orthogonal $\vec{\lambda}$ polarizations for each \vec{k} such that $\vec{\lambda} \cdot \vec{k} = 0$ and we have assumed that the universe is a very large box of volume V. The total energy in this wave solution is

$$E = \sum_{\vec{k}\vec{\lambda}} \frac{\omega^2}{2\pi c^2} \left| A_{\vec{k}\vec{\lambda}} \right|^2$$
(20.425)

How does this classical electromagnetic field interact with a quantum mechanical particle?

In general (no transverse gauge at this point), the classical Hamiltonian is

$$\hat{H} = \frac{\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{r},t)\right)^2}{2m} + e\phi(\vec{r},t) + V(\vec{r},t)$$
(20.426)

where $V(\vec{r}, t)$ represents all the other potentials seen by the particle.

We get to quantum mechanics via the standard substitutions

$$\vec{r} \to \vec{r}_{op}$$
 , $\vec{p} \to \vec{p}_{op} = \frac{\hbar}{i} \nabla$ (20.427)

Substituting, we get the Schrodinger equation for an electron in an electromagnetic field

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}(\vec{r},t)\right)^2 + e\phi(\vec{r},t) + V(\vec{r},t)\right]\psi(\vec{r},t)$$
(20.428)

20.7.2 Relation to Gauge Invariance

In order to have the Schrodinger equation invariant under a gauge transformation, the wave function has to change by a phase factor, i.e.,

$$\psi'(\vec{r},t) = e^{i\frac{e}{\hbar c}\chi(\vec{r},t)}\psi(\vec{r},t)$$
(20.429)

where $\chi(\vec{r}, t)$ is the some scalar function.

This means that the solutions of the gauge-transformed Schrodinger equation will still describe the same physical states.

The wave functions or state vectors differ by a phase factor that depends on space and time and thus, the invariance is LOCAL rather than GLOBAL (a phase factor independent of space and time).

It is then clear that it is NOT the canonical momentum $\hat{p} \rightarrow -i\hbar\nabla$ (whose expectation value is NOT gauge invariant), but the genuine kinetic momentum

$$\hat{p} - \frac{q}{c}\vec{A}(\hat{r},t)$$
 (20.430)

(whose expectation value IS gauge invariant), that represents a measurable quantity.

In any physical system, if the momentum operator \hat{p} appears, then it must always be replaced by

$$\psi'(\vec{r},t) = e^{i\frac{e}{\hbar c}\chi(\vec{r},t)}\psi(\vec{r},t)$$
(20.431)

if we turn on an electromagnetic fields. This is the only way to guarantee gauge invariance in quantum mechanics.

Quantum mechanics + electromagnetism requires *minimal coupling* for gauge invariance to be valid.

20.7.3 Interactions

We now write

$$\hat{H} = \hat{H}_0 + \hat{H}_{int}$$
 (20.432)

where

$$\hat{H}_0 = \frac{\vec{p}^2}{2m} + V(\vec{r}, t) \tag{20.433}$$

is the Hamiltonian in the absence of electromagnetic fields and

$$\hat{H}_{\rm int} = -\frac{e}{2mc} \left(\vec{p} \cdot \vec{A}(\vec{r}, t) + \vec{A}(\vec{r}, t) \cdot \vec{p} \right) + \frac{e^2}{2mc^2} \vec{A}^2(\vec{r}, t) + e\phi(\vec{r}, t)$$
(20.434)

is the operator giving the interaction between matter and radiation.

One must treat the term $\vec{p} \cdot \vec{A}(\vec{r},t) + \vec{A}(\vec{r},t) \cdot \vec{p}$ with care since $[x_i, p_j] = i\hbar \delta_{ij}$. In general, we can show that

$$\vec{p} \cdot \vec{A}(\vec{r},t) - \vec{A}(\vec{r},t) \cdot \vec{p} = -i\hbar \left(\nabla \cdot \vec{A}(\vec{r},t)\right)$$
(20.435)

which says that

$$\vec{p} \cdot \vec{A}(\vec{r},t) = \vec{A}(\vec{r},t) \cdot \vec{p} \text{ only when } \nabla \cdot \vec{A} = 0$$
 (20.436)

or when we are operating in the transverse gauge.

For multi-electron atoms we have

$$\hat{H} = \sum_{i=1}^{N} \frac{\left(\vec{p}_i - \frac{e}{c}\vec{A}(\vec{r}_i, t)\right)^2}{2m} + e\sum_{i=1}^{N} \phi(\vec{r}_i, t) + V$$
(20.437)

and

$$\hat{H}_{int} = \sum_{i=1}^{N} \left\{ -\frac{e}{2mc} \left(\vec{p}_i \cdot \vec{A}(\vec{r}_i, t) + \vec{A}(\vec{r}_i, t) \cdot \vec{p}_i \right) + \frac{e^2}{2mc^2} \vec{A}^2(\vec{r}_i, t) + e\phi(\vec{r}_i, t) \right\}$$
(20.438)

We now define a particle number density

$$\rho(\vec{r}) = \sum_{i} \delta(\vec{r} - \vec{r}_i) \tag{20.439}$$

and a current density

$$\vec{j}(\vec{r}) = \frac{1}{2} \sum_{i} \left(\frac{\vec{p}_i}{m} \delta(\vec{r} - \vec{r}_i) + \delta(\vec{r} - \vec{r}_i) \frac{\vec{p}_i}{m} \right)$$
(20.440)

where we constructed a symmetric combination of the terms so that the operator would be Hermitian.

These quantities imply that

$$\sum_{i} e\phi(\vec{r}_{i},t) = \sum_{i} \int d^{3}\vec{r} \, e\delta(\vec{r}-\vec{r}_{i})\phi(\vec{r},t) = \int d^{3}\vec{r} \, e\rho(\vec{r})\phi(\vec{r},t)$$
(20.441)

where $\phi(\vec{r}, t) \neq \text{operator}$ (all operators are in $\rho(\vec{r})$) and

$$\int d^3 \vec{r} \rho(\vec{r}) = N = \text{ total number of particles}$$
(20.442)

Finally, we have

$$\sum_{i=1}^{N} \left\{ -\frac{e}{2mc} \left(\vec{p}_i \cdot \vec{A}(\vec{r}_i, t) + \vec{A}(\vec{r}_i, t) \cdot \vec{p}_i \right) \right\} = -\frac{e}{c} \int d^3 \vec{r} \vec{j}(\vec{r}) \cdot \vec{A}(\vec{r}, t)$$
(20.443)

Since

$$\vec{v}_i = \frac{\vec{p}_i}{m} - \frac{e}{mc}\vec{A} \tag{20.444}$$

when an electromagnetic field is present, the true current operator is

$$\vec{J}(\vec{r}) = \vec{j}(\vec{r}) - \frac{e}{mc}\vec{A}(\vec{r},t)\rho(\vec{r}) = (\text{paramagnetic} + \text{diamagnetic}) \text{ currents}$$
(20.445)

and therefore,

$$\hat{H}_{\rm int} = \int d^3 \vec{r} \left[-\frac{e}{c} \vec{j}(\vec{r}) \cdot \vec{A}(\vec{r},t) + \frac{e^2}{2mc^2} \rho(\vec{r}) \vec{A}^2(\vec{r},t) + e\phi(\vec{r},t)\rho(\vec{r}) \right] \quad (20.446)$$

20.7.4 Induced Absorption and Emission

We will now use the transverse gauge, which says that the $\phi(\vec{r}, t)$ term is zero. We also assume that the radiation fields are small compared to the fields inside the atom, i.e., $|\vec{A}| \ll e^2/a_0$, which implies that we can neglect the \vec{A}^2 term compared to the $\vec{j} \cdot \vec{A}$ term. Therefore, we have

$$\hat{H}_{int} = -\frac{e}{c} \int d^3 \vec{r} \, \vec{j}(\vec{r}) \cdot \vec{A}(\vec{r},t)$$
(20.447)

For \vec{A} as a linear superposition of monochromatic plane waves we then have

$$\begin{split} \hat{H}_{int} &= -\frac{e}{c} \int d^{3}\vec{r} \left(\frac{1}{2} \sum_{i} \left(\frac{\vec{p}_{i}}{m} \delta(\vec{r} - \vec{r}_{i}) + \delta(\vec{r} - \vec{r}_{i}) \frac{\vec{p}_{i}}{m} \right) \right) \\ & \times \left(\sum_{\vec{k}\vec{\lambda}} \left[A_{\vec{k}\vec{\lambda}} \vec{\lambda} \frac{e^{i\vec{k}\cdot\vec{r}-i\omega t}}{\sqrt{V}} + A_{\vec{k}\vec{\lambda}}^{*} \vec{\lambda}^{*} \frac{e^{-i\vec{k}\cdot\vec{r}+i\omega t}}{\sqrt{V}} \right] \right) \\ &= -\frac{e}{2c\sqrt{V}} \sum_{\vec{k}\vec{\lambda}} \sum_{i} \left(\begin{array}{c} A_{\vec{k}\vec{\lambda}} \vec{\lambda} \frac{\vec{p}_{i}}{m} e^{i\vec{k}\cdot\vec{r}_{i}-i\omega t} + A_{\vec{k}\vec{\lambda}}^{*} \vec{\lambda}^{*} \frac{\vec{p}_{i}}{m} e^{-i\vec{k}\cdot\vec{r}_{i}+i\omega t}}{+A_{\vec{k}\vec{\lambda}} \vec{\lambda} e^{i\vec{k}\cdot\vec{r}_{i}-i\omega t} \frac{\vec{p}_{i}}{m} + A_{\vec{k}\vec{\lambda}}^{*} \vec{\lambda}^{*} e^{-i\vec{k}\cdot\vec{r}_{i}+i\omega t} \frac{\vec{p}_{i}}{m}}{+A_{\vec{k}\vec{\lambda}} \vec{\lambda} e^{-i\omega t} + A_{\vec{k}\vec{\lambda}}^{*} \vec{j}_{\vec{k}} \cdot \vec{\lambda}^{*} e^{i\omega t}} \right] \\ &= -\frac{e}{c\sqrt{V}} \sum_{\vec{k}\vec{\lambda}} \left[A_{\vec{k}\vec{\lambda}} \vec{j}_{-\vec{k}} \cdot \vec{\lambda} e^{-i\omega t} + A_{\vec{k}\vec{\lambda}}^{*} \vec{j}_{\vec{k}} \cdot \vec{\lambda}^{*} e^{i\omega t} \right] \tag{20.448} \end{split}$$

where

$$\vec{j}_{\vec{k}} = \frac{1}{2} \sum_{i} \left(\frac{\vec{p}_{i}}{m} e^{-i\vec{k}\cdot\vec{r}_{i}} + e^{-i\vec{k}\cdot\vec{r}_{i}} \frac{\vec{p}_{i}}{m} \right) = \int d^{3}\vec{r} e^{-i\vec{k}\cdot\vec{r}} \vec{j}(\vec{r})$$
(20.449)

As we saw in the discussion of time-dependent perturbation theory for a harmonic perturbation, the $e^{-i\omega t}$ term implies an absorption of radiation process and the $e^{i\omega t}$ term implies and emission of radiation process. Following the same steps as that case, we have for the absorption transition rate

$$\Gamma^{abs}_{0 \to n; \vec{k}\vec{\lambda}} = \frac{2\pi}{\hbar} \delta(\varepsilon_n - \varepsilon_0 - \hbar\omega) \frac{e^2}{Vc^2} \left| A_{\vec{k}\vec{\lambda}} \right|^2 \left| \langle n | \vec{j}_{\vec{k}} \cdot \vec{\lambda} | 0 \rangle \right|^2 \tag{20.450}$$

To find the total rate of transition we must sum over \vec{k} and $\vec{\lambda}$ (2 polarizations for each \vec{k}) to get

$$\Gamma_{0 \to n}^{abs} = \frac{2\pi}{\hbar V} \sum_{\vec{k}\vec{\lambda}} \delta(\varepsilon_n - \varepsilon_0 - \hbar\omega) \frac{e^2}{c^2} \left| A_{\vec{k}\vec{\lambda}} \right|^2 \left| \langle n | \vec{j}_{-\vec{k}} \cdot \vec{\lambda} | 0 \rangle \right|^2$$
(20.451)

Now we can write

$$\frac{1}{V}\sum_{\vec{k}} \to \int \frac{k^2 dk d\Omega}{(2\pi)^3} = \int \frac{\omega^2 d\omega d\Omega}{(2\pi c)^3}$$
(20.452)

so that

$$\Gamma_{0 \to n}^{abs} = \frac{2\pi e^2}{\hbar^2 c^2} \frac{\omega^2}{2\pi c^3} \int d\Omega \sum_{\vec{\lambda}} \left| A_{\vec{k}\vec{\lambda}} \right|^2 \left| \langle n | \vec{j}_{\vec{k}} \cdot \vec{\lambda} | 0 \rangle \right|^2 \tag{20.453}$$

where

$$\omega = \frac{\varepsilon_n - \varepsilon_0}{\hbar} \text{ (from the } \delta - \text{ function)}$$
(20.454)

If the incident light beam subtends a solid angle $d\Omega$ and it is polarized with polarization vector $\vec{\lambda}$, then the total rate of energy transport in the beam is the time average of the Poynting vector which is given by

$$\frac{1}{V}\sum_{\vec{k}}\frac{\omega^2}{2\pi c}\left|A_{\vec{k}\vec{\lambda}}\right|^2 = d\Omega \int d\omega \frac{\omega^4}{(2\pi c)^4}\left|A_{\vec{k}\vec{\lambda}}\right|^2 \tag{20.455}$$

Now

$$I(\omega) = d\Omega \frac{\omega^4}{(2\pi c)^4} \left| A_{\vec{k}\vec{\lambda}} \right|^2$$

= intensity of the incident beam per unit frequency (20.456)

In a similar way

$$\Gamma_{n \to 0}^{ind \; emis} = \frac{4\pi^2 e^2}{\hbar^2 c\omega^2} I(\omega) \left| \langle n | \, \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \, | 0 \rangle \right|^2 \tag{20.457}$$

Since

$$\langle n | \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* | 0 \rangle = \langle n | \vec{j}_{-\vec{k}} \cdot \vec{\lambda} | 0 \rangle^*$$
(20.458)

we have

$$\Gamma_{0 \to n}^{abs} = \Gamma_{n \to 0}^{ind \; emis} \tag{20.459}$$

(this is the origin of the Einstein A and B coefficients).

In the absorption process, the absorption of one photon of energy $\hbar\omega = \varepsilon_n - \varepsilon_0$ causes an upward transition. The electron gains energy and the electromagnetic field loses energy. Induced emission is just the opposite.

Now a photon of frequency ω and energy $\hbar\omega$ and therefore, the total energy in the incident beam is

$$E = \sum_{\vec{k}\vec{\lambda}} \hbar\omega N_{\vec{k}\vec{\lambda}} \tag{20.460}$$

where $N_{\vec{k}\vec{\lambda}}$ = the number of photons in the $(\vec{k},\vec{\lambda})$ mode in the beam. But we already have

$$E = \sum_{\vec{k}\vec{\lambda}} \frac{\omega^2}{2\pi c^2} \left| A_{\vec{k}\vec{\lambda}} \right|^2 \tag{20.461}$$

which says that

$$\left|A_{\vec{k}\vec{\lambda}}\right|^2 = \frac{2\pi\hbar c^2}{\omega} N_{\vec{k}\vec{\lambda}} \tag{20.462}$$

and thus

$$\Gamma_{0 \to n}^{abs} = \Gamma_{n \to 0}^{ind \; emis} = \sum_{\vec{k}\vec{\lambda}} \frac{4\pi^2 e^2}{\omega V} \delta(\varepsilon_n - \varepsilon_0 - \hbar\omega) \left| \langle n | \, \vec{j}_{-\vec{k}} \cdot \vec{\lambda} \, | 0 \rangle \right|^2 N_{\vec{k}\vec{\lambda}} \tag{20.463}$$

20.7.5 Quantized Radiation Field and Spontaneous Emission

Up to this point we have been treating the electromagnetic field classically as a wave. We have mentioned the idea of photons, but have not created any formal quantum mechanical structure to describe them, i.e., we have been considering what happens to the atom and ignoring what is happening to the EM field during these processes.

To bring out the structure of the theory in terms of photons, we must now describe these processes in terms of state vectors, such that, in the absorption process the atom makes a transition from $|0\rangle \rightarrow |n\rangle$ while the electromagnetic field makes a transition from an initial state to a state with *one less photon* (it has been absorbed).

All of our development so far has involved what is physically called an incoherent beam of light.

We related $|A_{\vec{k}\vec{\lambda}}|$ and $N_{\vec{k}\vec{\lambda}}$ so that knowledge of the $N_{\vec{k}\vec{\lambda}}$ clearly does not imply any information about the relative phases of the $A_{\vec{k}\vec{\lambda}}$ which is the meaning of the term incoherent.

An incoherent beam, therefore, is completely specified by the photon numbers, i.e., the $N_{\vec{k}\vec{\lambda}}$. It is in this sense that we can write the initial state(normalized) of the electromagnetic field as

$$|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, \dots, N_{\vec{k}\vec{\lambda}}, \dots \rangle$$
(20.464)

where, as before, the $N_{\vec{k}\vec{\lambda}}$ = the number of photons in the mode $(\vec{k},\vec{\lambda})$.

Any two of these states are orthogonal if they differ in the number of photons in any mode.

The final state of the electromagnetic field after photon absorption of a photon in the mode $(\vec{k}, \vec{\lambda})$ is

$$|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, \dots, N_{\vec{k}\vec{\lambda}} - 1, \dots \rangle$$
(20.465)

We assume that there exists some \hat{H}_{int} that causes both transitions (atom and electromagnetic field) as it couples the electromagnetic field to matter. We define

initial state =
$$|0\rangle |N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, \dots, N_{\vec{k}\vec{\lambda}}, \dots)$$
 (20.466)

final state =
$$|n\rangle |N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, \dots, N_{\vec{k}\vec{\lambda}} - 1, \dots)$$
 (20.467)

so that

$$E_{initial} = \varepsilon_0 + \sum_{\vec{k}\,\prime\vec{\lambda}\,\prime} \hbar c k' N_{\vec{k}\,\prime\vec{\lambda}\,\prime} \tag{20.468}$$

$$E_{final} = \varepsilon_n + \sum_{\vec{k}\,'\vec{\lambda}\,'} \hbar c k' N_{\vec{k}\,'\vec{\lambda}\,'} - \hbar c k \tag{20.469}$$

The transition rate between the two states is given by Fermi's golden rule as

$$\frac{2\pi}{\hbar}\delta(\varepsilon_n - \varepsilon_0 - \hbar\omega) \left| \langle final | \hat{H}_{int} | initial \rangle \right|^2 \tag{20.470}$$

This must be the same as our earlier result (20.463) which implies that we must have

$$\begin{aligned} \left| \langle final | \hat{H}_{int} | initial \rangle \right|^2 &= \frac{e^2}{Vc^2} \left| A_{\vec{k}\vec{\lambda}} \right|^2 \left| \langle n | \vec{j}_{-\vec{k}} \cdot \vec{\lambda} | 0 \rangle \right|^2 \\ &= \frac{e^2}{Vc^2} \frac{2\pi\hbar c^2}{\omega} N_{\vec{k}\vec{\lambda}} \left| \langle n | \vec{j}_{-\vec{k}} \cdot \vec{\lambda} | 0 \rangle \right|^2 \end{aligned} \tag{20.471}$$

This implies that as yet undetermined operator \hat{H}_{int} must have the following properties:

- 1. it must include a part $\vec{j}_{-\vec{k}}\cdot\vec{\lambda}$ that acts on the atom
- 2. it must have a part that decreases the number of photons in the $(\vec{k},\vec{\lambda})$ mode by 1
- 3. it must be Hermitian

One way of doing this is to write

$$\hat{H}_{int} = \frac{e}{c\sqrt{V}} \sum_{\vec{k}\,'\vec{\lambda}\,'} \left(\vec{j}_{-\vec{k}\,'} \cdot \vec{\lambda}\,' A^{(op)}_{\vec{k}\,'\vec{\lambda}\,'} + \vec{j}_{\vec{k}\,'} \cdot \vec{\lambda}\,'^* A^{(op)+}_{\vec{k}\,'\vec{\lambda}\,'} \right)$$
(20.472)

where $A_{\vec{k}\vec{\lambda}}^{(op)}$ reduces the number of photons in the $(\vec{k},\vec{\lambda})$ mode by 1. It is a photon in mode $(\vec{k},\vec{\lambda})$ annihilation operator.

The second term is required to make \hat{H}_{int} Hermitian. Using this model we then have

$$\begin{aligned} \langle final | \hat{H}_{int} | initial \rangle \\ &= \langle n; N_{\vec{k}_1 \vec{\lambda}_1}, N_{\vec{k}_2 \vec{\lambda}_2}, \dots, N_{\vec{k} \vec{\lambda}} - 1, \dots | \hat{H}_{int} | 0; N_{\vec{k}_1 \vec{\lambda}_1}, N_{\vec{k}_2 \vec{\lambda}_2}, \dots, N_{\vec{k} \vec{\lambda}}, \dots \rangle \\ &= -\frac{e}{c} \langle n | \vec{j}_{-\vec{k}} \cdot \vec{\lambda} | 0 \rangle \\ &\times \langle N_{\vec{k}_1 \vec{\lambda}_1}, N_{\vec{k}_2 \vec{\lambda}_2}, \dots, N_{\vec{k} \vec{\lambda}} - 1, \dots | A_{\vec{k} \vec{\lambda}}^{(op)} | N_{\vec{k}_1 \vec{\lambda}_1}, N_{\vec{k}_2 \vec{\lambda}_2}, \dots, N_{\vec{k} \vec{\lambda}}, \dots \rangle \\ \end{aligned}$$
(20.473)

For agreement with the earlier result we must have

$$\left\langle N_{\vec{k}_{1}\vec{\lambda}_{1}}, N_{\vec{k}_{2}\vec{\lambda}_{2}}, \dots, N_{\vec{k}\vec{\lambda}} - 1, \dots \right| A_{\vec{k}\vec{\lambda}}^{(op)} \left| N_{\vec{k}_{1}\vec{\lambda}_{1}}, N_{\vec{k}_{2}\vec{\lambda}_{2}}, \dots, N_{\vec{k}\vec{\lambda}}, \dots \right\rangle$$

$$= \sqrt{\frac{2\pi\hbar c^{2}}{\omega}} \sqrt{N_{\vec{k}\vec{\lambda}}}$$

$$(20.474)$$

This matrix element of $A^{(op)}_{\vec{k}\vec{\lambda}}$ corresponds to the $A_{\vec{k}\vec{\lambda}}$ term in the classical field picture.

The matrix element implies that

which says that $A_{\vec{k}\vec{\lambda}}^{(op)+}$ is an operator that increases the number of photons in the $(\vec{k},\vec{\lambda})$ mode by 1. It is a photon in mode $(\vec{k},\vec{\lambda})$ creation operator. We thus have

$$\begin{aligned}
A_{\vec{k}\vec{\lambda}}^{(op)} &| N_{\vec{k}_{1}\vec{\lambda}_{1}}, N_{\vec{k}_{2}\vec{\lambda}_{2}}, ..., N_{\vec{k}\vec{\lambda}}, ... \rangle \\
&= \sqrt{\frac{2\pi\hbar c^{2}}{\omega}} \sqrt{N_{\vec{k}\vec{\lambda}}} \left| N_{\vec{k}_{1}\vec{\lambda}_{1}}, N_{\vec{k}_{2}\vec{\lambda}_{2}}, ..., N_{\vec{k}\vec{\lambda}} - 1, ... \right\rangle \\
A_{\vec{k}\vec{\lambda}}^{(op)+} &| N_{\vec{k}_{1}\vec{\lambda}_{1}}, N_{\vec{k}_{2}\vec{\lambda}_{2}}, ..., N_{\vec{k}\vec{\lambda}}, ... \rangle
\end{aligned}$$
(20.476)

$$= \sqrt{\frac{2\pi\hbar c^2}{\omega}} \sqrt{N_{\vec{k}\vec{\lambda}} + 1} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, \dots, N_{\vec{k}\vec{\lambda}} + 1, \dots \right\rangle$$
(20.477)

This behavior is identical (aside from the $\sqrt{2\pi\hbar c^2/\omega}$ factor) to that of the \hat{a} and \hat{a}^+ operators in the harmonic oscillator problem.

This model gives a quantum mechanical picture of the electromagnetic radiation field as an infinite number of *harmonic oscillators* - one per mode and the quanta associated with these oscillators are photons.

If we define a Hermitian electromagnetic field operator as

$$\vec{A}^{(op)}(\vec{r}) = \sum_{\vec{k}\vec{\lambda}} \left[A^{(op)}_{\vec{k}\vec{\lambda}} \vec{\lambda} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} + A^{(op)+}_{\vec{k}\vec{\lambda}} \vec{\lambda}^* \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \right]$$
(20.478)

we have

$$\hat{H}_{int} = \int d^3 \vec{r} \left[-\frac{e}{c} \vec{j}(\vec{r}) \cdot \vec{A}^{(op)}(\vec{r}) + \frac{e^2}{2mc^2} \rho(\vec{r}) \left(\vec{A}^{(op)}(\vec{r}) \right)^2 \right]$$
(20.479)

In the interaction representation $\vec{A}^{(op)}(\vec{r},t)$ has the time dependence

$$\vec{A}^{(op)}(\vec{r},t) = e^{\frac{i}{\hbar}\hat{H}_{em}t}\vec{A}^{(op)}(\vec{r})e^{-\frac{i}{\hbar}\hat{H}_{em}t}$$
(20.480)

where \hat{H}_{em} = Hamiltonian for free radiation. We then have

$$\hat{H}_{em} = \frac{1}{8\pi} \int d^3 \vec{r} \left(\vec{\varepsilon}^2 + \vec{B}^2 \right) = \sum_{\vec{k}\vec{\lambda}} \hbar ck \left(A^{(op)+}_{\vec{k}\vec{\lambda}} A^{(op)}_{\vec{k}\vec{\lambda}} + \frac{1}{2} \right)$$
(20.481)

The operator algebra similarity to the \hat{a} and \hat{a}^+ problem then allows us to write

$$\left[A^{(op)}_{\vec{k}\vec{\lambda}}, A^{(op)+}_{\vec{k}'\vec{\lambda}'}\right] = \frac{2\pi\hbar c^2}{\omega} \delta_{\vec{k}\vec{k}'} \delta_{\vec{\lambda}\vec{\lambda}'} \quad , \quad \left[A^{(op)}_{\vec{k}\vec{\lambda}}, A^{(op)}_{\vec{k}'\vec{\lambda}'}\right] = 0 \tag{20.482}$$

and

$$\left|N_{\vec{k}_{1}\vec{\lambda}_{1}}, N_{\vec{k}_{2}\vec{\lambda}_{2}}, ..., N_{\vec{k}\vec{\lambda}}, ...\right\rangle = \frac{1}{\sqrt{N_{\vec{k}\vec{\lambda}}!}} \left(A_{\vec{k}\vec{\lambda}}^{(op)+}\right)^{N_{\vec{k}\vec{\lambda}}} \left|N_{\vec{k}_{1}\vec{\lambda}_{1}}, N_{\vec{k}_{2}\vec{\lambda}_{2}}, ..., 0, ...\right\rangle$$
(20.483)

and $\hat{H} = \hat{H}_0 + \hat{H}_{em} + \hat{H}_{int}$ where $\hat{H}_0 =$ Hamiltonian for the electrons.

We then have

$$e^{\frac{i}{\hbar}\hat{H}_{em}t}A_{\vec{k}\vec{\lambda}}^{(op)}e^{-\frac{i}{\hbar}\hat{H}_{em}t}\left|....,N_{\vec{k}\vec{\lambda}},....\right\rangle$$

$$= e^{\frac{i}{\hbar}\hat{H}_{em}t}A_{\vec{k}\vec{\lambda}}^{(op)}e^{-i(N_{\vec{k}\vec{\lambda}}+\frac{1}{2})t}\left|....,N_{\vec{k}\vec{\lambda}},....\right\rangle$$

$$= e^{\frac{i}{\hbar}\hat{H}_{em}t}e^{-i(N_{\vec{k}\vec{\lambda}}+\frac{1}{2})t}\sqrt{N_{\vec{k}\vec{\lambda}}}\left|....,N_{\vec{k}\vec{\lambda}}-1,....\right\rangle$$

$$= e^{i(N_{\vec{k}\vec{\lambda}}-1+\frac{1}{2})t}e^{-i(N_{\vec{k}\vec{\lambda}}+\frac{1}{2})t}\sqrt{N_{\vec{k}\vec{\lambda}}}\left|....,N_{\vec{k}\vec{\lambda}}-1,....\right\rangle$$

$$= e^{-ickt}A_{\vec{k}\vec{\lambda}}^{(op)}\left|....,N_{\vec{k}\vec{\lambda}},....\right\rangle$$
(20.484)

or

$$e^{\frac{i}{\hbar}\hat{H}_{em}t}A^{(op)}_{\vec{k}\vec{\lambda}}e^{-\frac{i}{\hbar}\hat{H}_{em}t} = e^{-ickt}A^{(op)}_{\vec{k}\vec{\lambda}}$$
(20.485)

and similarly

$$e^{\frac{i}{\hbar}\hat{H}_{em}t}A^{(op)+}_{\vec{k}\vec{\lambda}}e^{-\frac{i}{\hbar}\hat{H}_{em}t} = e^{ickt}A^{(op)+}_{\vec{k}\vec{\lambda}}$$
(20.486)

Putting this all together we have

$$\vec{A}^{(op)}(\vec{r},t) = \sum_{\vec{k}\vec{\lambda}} \left[A^{(op)}_{\vec{k}\vec{\lambda}} \vec{\lambda} \frac{e^{i\vec{k}\cdot\vec{r}-i\omega t}}{\sqrt{V}} + A^{(op)+}_{\vec{k}\vec{\lambda}} \vec{\lambda}^* \frac{e^{-i\vec{k}\cdot\vec{r}+i\omega t}}{\sqrt{V}} \right]$$
(20.487)

By construction, we have forced the quantum mechanical description of absorption of the electromagnetic field in terms of the photon to be identical to the description in terms of the classical electromagnetic field for the induced absorption process.

We now apply the formalism to the emission process. This corresponds to the transition between the states

initial state =
$$|0\rangle |N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, \dots, N_{\vec{k}\vec{\lambda}}, \dots\rangle$$
 (20.488)

final state =
$$|n\rangle |N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, \dots, N_{\vec{k}\vec{\lambda}} + 1, \dots)$$
 (20.489)

so that

$$E_{initial} = \varepsilon_0 + \sum_{\vec{k}\,\prime\vec{\lambda}\,\prime} \hbar c k' N_{\vec{k}\,\prime\vec{\lambda}\,\prime} \tag{20.490}$$

$$E_{final} = \varepsilon_n + \sum_{\vec{k}\,'\vec{\lambda}\,'} \hbar c k' N_{\vec{k}\,'\vec{\lambda}\,'} + \hbar c k \tag{20.491}$$

The transition rate is

$$\frac{2\pi}{\hbar}\delta(\varepsilon_n - \varepsilon_0 - \hbar ck) \left| \left\langle 0; \dots, N_{\vec{k}\vec{\lambda}} + 1, \dots, \left| \hat{H}_{\text{int}} \right| n; \dots, N_{\vec{k}\vec{\lambda}}, \dots \right\rangle \right|^2 \qquad (20.492)$$

where

$$\begin{aligned} \left\langle 0; \dots, N_{\vec{k}\vec{\lambda}} + 1, \dots, \left| \hat{H}_{int} \right| n; \dots, N_{\vec{k}\vec{\lambda}}, \dots \right\rangle \\ &= -\frac{e}{c\sqrt{V}} \left\langle 0 \right| \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \left| n \right\rangle \left\langle \dots, N_{\vec{k}\vec{\lambda}} + 1, \dots, \left| A_{\vec{k}\vec{\lambda}}^{(op)+} \right| \dots, N_{\vec{k}\vec{\lambda}}, \dots \right\rangle \\ &= -\frac{e}{c} \sqrt{\frac{2\pi\hbar c}{\omega V}} \left\langle 0 \right| \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \left| n \right\rangle \sqrt{N_{\vec{k}\vec{\lambda}} + 1}$$
(20.493)

We no longer have any features that are unknown and hence adjustable. Forcing agreement with induced absorption makes the results for the emission process a prediction!

We get

$$\Gamma_{n\to0;\vec{k}\vec{\lambda}}^{emis} = \frac{4\pi^2 e^2}{\omega V} \delta(\varepsilon_n - \varepsilon_0 - \hbar ck) \left| \langle 0 | \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* | n \rangle \right|^2 \left(N_{\vec{k}\vec{\lambda}} + 1 \right) \neq \Gamma_{0\to n;\vec{k}\vec{\lambda}}^{abs} \quad (20.494)$$

which disagrees with the classical field result but agrees with experiment.

The $N_{\vec{k}\vec{\lambda}}$ part corresponds to the classical result.

The +1 part is a purely quantum mechanical effect.

This term implies that there is an emission process that can take place even if there is *no external field* present.

This process is called *spontaneous emission*. A clear victory for the quantum approach.

20.8 Problems

20.8.1 Dirac Spinors

The Dirac spinors are (with E = $\sqrt{\vec{p}^2+m^2})$

$$u(p,s) = \frac{\not p + m}{\sqrt{E + m}} \begin{pmatrix} \varphi_s \\ 0 \end{pmatrix} \quad , \quad v(p,s) = \frac{-\not p + m}{\sqrt{E + m}} \begin{pmatrix} 0 \\ \chi_s \end{pmatrix}$$

where $\not p = \gamma^{\mu} p_{\mu}$, $\varphi_s(s = \pm 1/2)$ are orthonormalized 2-spinors and similarly for χ_s . Prove(using $\bar{u} = u^+ \gamma^0$, etc):

(a)
$$\bar{u}(p.s)u(p.s') = -\bar{v}(p,s)v(p,s') = 2m\delta_{ss'}$$

- (b) $\bar{v}(p,s)u(p,s') = 0$
- (c) $\bar{u}(p,s)\gamma^0 u(p,s') = 2E\delta_{ss'}$
- (d) $\sum_{s} u(p.s)\overline{u}(p,s) = p + m$
- (e) $\sum_{s} v(p.s) \overline{v}(p,s) = p m$
- (f) $\bar{u}(p,s)\gamma^{\mu}u(p',s') = 2E\delta_{ss'} = \frac{1}{2m}\bar{u}(p,s)\left[(p+p')^{\mu} + i\sigma^{\mu\nu}(p-p')_{\nu}\right]u(p',s')$ (*The Gordon Identity*)

20.8.2 Lorentz Transformations

In a Lorentz transformation $x' = \Lambda x$ the Dirac wave function transforms as $\psi'(x') = S(\Lambda)\psi(x)$, where $S(\Lambda)$ is a 4×4 matrix.

(a) Show that the Dirac equation is invariant in form, i.e., $(i\gamma^{\mu}\partial'_{\mu} - m)\psi'(x') = 0$, provided

$$S^{-1}(\Lambda)\gamma^{\mu}S(\Lambda) = \Lambda^{\mu}_{\ \nu}\gamma^{\nu}$$

(b) For an infinitesimal transformation $\Lambda^{\mu}_{\ \nu} = g^{\mu}_{\ \nu} + \delta \omega^{\mu}_{\ \nu}$, where $\delta \omega_{\mu\nu} = -\delta \omega_{\nu\mu}$. The spin dependence of $S(\Lambda)$ is given by $I - i\sigma_{\mu\nu}\delta\omega^{\mu\nu}/4$. Show that $\sigma_{\mu\nu} = i[\gamma_{\mu}, \gamma_{nu}]$ satisfies the equation in part (a). For finite transformations we then have $S(\Lambda) = e^{-i\sigma_{\mu\nu}\omega^{\mu\nu}/4}$.

20.8.3 Dirac Equation in 1+1 Dimensions

Consider the Dirac equation in 1 + 1 Dimensions (i.e., one space and one time dimension):

$$\left(i\gamma^0\frac{\partial}{\partial x^0} + i\gamma^1\frac{\partial}{\partial x^1} - m\right)\psi(x) = 0$$

- (a) Find a 2 × 2 matrix representation of γ^0 and γ^1 which satisfies $\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu}$ and has correct hermiticity. What is the physical reason that ψ can have only two components in 1 + 1 dimensions?
- (b) Find the representation of $\gamma_5 = \gamma^0 \gamma^1$, $\gamma_5 \gamma^{\mu}$ and $\sigma^{\mu\nu} = \frac{1}{2}i [\gamma^{\mu}, \gamma^{\nu}]$. Are they independent? Define a minimal set of matrices which form a complete basis.
- (c) Find the plane wave solutions $\psi_+(x) = u(p^1)e^{-ip\cdot x}$ and $\psi_-(x) = v(p^1)e^{ip\cdot x}$ in 1 + 1 dimensions, normalized to $\bar{u}u = -\bar{v}v = 2m$ (where $\bar{u} = u^+\gamma^0$).

20.8.4 Trace Identities

Prove the following trace identities for Dirac matrices using only their property $\{\gamma^{\mu}, \gamma^{\nu}\} = g^{\mu\nu}$ (i.e., do not use a specific matrix representation)

(a) $Tr(\gamma^{\mu}) = 0$

- (b) $Tr(\gamma^{\mu}\gamma^{\nu}) = 4g^{\mu\nu}$
- (c) $Tr(\gamma^{\mu}\gamma^{\nu}\gamma^{\rho}) = 0$
- (d) $Tr(\gamma^{\mu}\gamma^{\nu}\gamma^{\rho}\gamma^{\sigma}) = 4g^{\mu\nu}g^{\rho\sigma} 4g^{\mu\rho}g^{\nu\sigma} + 4g^{\mu\sigma}g^{\nu\rho}$
- (e) $Tr(\gamma_5) = 0$ where $\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$

20.8.5 Right- and Left-Handed Dirac Particles

The right (R) and left (L) -handed Dirac particles are defined by the projections

$$\psi_R(x) = \frac{1}{2}(1+\gamma_5)\psi(x)$$
, $\psi_L(x) = \frac{1}{2}(1-\gamma_5)\psi(x)$

In the case of a massless particle (m=0):

(a) Show that the Dirac equation $(i\partial - eA)\psi = 0$ does not couple $\psi_R(x)$ to $\psi_L(x)$, i.e., they satisfy independent equations. Specifically, show that in the chiral representation of the Dirac matrices

$$\gamma^{0} = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix} \quad , \quad \gamma = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix}$$

we have

$$\psi = \begin{pmatrix} \phi_R \\ \phi_L \end{pmatrix} e^{-ip \cdot x}$$

i.e., that the lower(upper) two components of $\psi_R(\psi_L)$ vanish.

(b) For the free Dirac equation $(A^{\mu} = 0)$ show that ϕ_R and ϕ_L are eigenstates of the helicity operator $\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{p}$ with positive and negative helicity, respectively, for plane wave states with $p^0 > 0$.

20.8.6 Gyromagnetic Ratio for the Electron

(a) Reduce the Dirac equation $(i\partial - eA - m)\psi = 0$ by multiplying it with $(i\partial - eA + m)\psi = 0$ to the form

$$\left[(i\partial - eA)^2 - \frac{e}{2}\sigma^{\mu\nu}F_{\mu\nu} - m^2\right]\psi = 0$$

where $\sigma^{\mu\nu} = \frac{i}{2} [\gamma^{\mu}, \gamma^{\nu}]$ and the field strength $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$.

(b) Show that the dependence in the magnetic field $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ in the spindependent term $\sigma^{\mu\nu}F_{\mu\nu}$ is of the form $-(ge/2m)\frac{1}{2}\boldsymbol{\Sigma}\cdot\boldsymbol{B}$ when the kinetic energy is normalized to $-\nabla^2/2m$ ($\boldsymbol{\Sigma} = \gamma_5\gamma^0\boldsymbol{\gamma}$ is the spin matrix). Determine the value of the gyromagnetic ration g for the electron.

20.8.7 Dirac \rightarrow Schrodinger

Reduce type Dirac equation $(i\partial - eA - m)\psi = 0$ for the Hydrogen atom $(A^0 = -Ze/4\pi r, A = 0)$ to the standard Schrodinger equation

$$i\frac{\partial}{\partial t}\Psi(t, boldsymbolx) = \left(-\frac{\nabla^2}{2m} + eA^0\right)\Psi(t, boldsymbolx)$$

in the non-relativistic limit, where $|\mathbf{p}|$, $A^0 \ll m$. **HINT**: You may start from the reduced form of the Dirac equation in Problem 20.6(a). Extract the leading time dependence by writing $\psi(x) = \Psi(t, \mathbf{x})e^{-imt}$.

20.8.8 Positive and Negative Energy Solutions

Positive energy solutions of the Dirac equation correspond to the 4-vector current $J^{\mu} = 2p^{\mu} = 2(E, \vec{p}), E > 0$. Show that the negative energy solutions correspond to the current $J^{\mu} = -2(E, \vec{p}) = -2(|E|, -\vec{p}) = -2p^{\mu}, E < 0$.

20.8.9 Helicity Operator

(1) Show that the helicity operator commutes with the Hamiltonian:

$$\left[\vec{\Sigma} \cdot \hat{\boldsymbol{p}}, \boldsymbol{H} \right] = 0$$

(2) Show explicitly that the solutions to the Dirac equation are eigenvectors of the helicity operator:

$$\left[\vec{\Sigma} \cdot \hat{\boldsymbol{p}} \right] \Psi = \pm \Psi$$

20.8.10 Non-Relativisitic Limit

Consider

$$\Psi = \begin{pmatrix} \boldsymbol{u}_A \\ \boldsymbol{u}_B \end{pmatrix}$$

to be a solution of the Dirac equation where u_A and u_B are two-component spinors. Show that in the non-relativistic limit $u_B \sim \beta = v/c$.

20.8.11 Gyromagnetic Ratio

Show that in the non-relativisitc limit the motion of a spin 1/2 fermion of charge e in the presence of an electromagnetic field $A^{\mu} = (A^0, \vec{A})$ is described by

$$\left[\frac{(\vec{p}-e\vec{A})^2}{2m} - \frac{e}{2m}\vec{\sigma}\cdot\vec{B} + eA^0\right]\chi = E\chi$$

where \vec{B} is the magnetic field, σ^i are the Pauli matrices and $E = p^0 - m$. Identify the g-factor of the fermion and show that the Dirac equation predicts the correct gyromagnetic ratio for the fermion. To write down the Dirac equation in the presence of an electromagnetic field substitute: $p^{\mu} \rightarrow p^{\mu} - eA^{\mu}$.

20.8.12 Properties of γ_5

Show that:

- (a) $\overline{\Psi}\gamma_5\Psi$ is a pseudoscalar.
- (b) $\bar{\Psi}\gamma_5\gamma^{\mu}\Psi$ is an axial vector.

20.8.13 Lorentz and Parity Properties

Comment on the Lorentz and parity properties of the quantities:

- (a) $\bar{\Psi}\gamma_5\gamma^\mu\Psi\bar{\Psi}\gamma_\mu\Psi$
- (b) $\bar{\Psi}\gamma_5\Psi\bar{\Psi}\gamma_5\Psi$
- (c) $\bar{\Psi}\Psi\bar{\Psi}\gamma_5\Psi$
- (d) $\bar{\Psi}\gamma_5\gamma^\mu\Psi\bar{\Psi}\gamma_5\gamma_\mu\Psi$
- (e) $\bar{\Psi}\gamma^{\mu}\Psi\bar{\Psi}\gamma_{\mu}\Psi$

20.8.14 A Commutator

Explicitly evaluate the commutator of the Dirac Hamiltonian with the orbital angular momentum operator \hat{L} for a free particle.

20.8.15 Solutions of the Klein-Gordon equation

Let $\phi(\vec{r}, t)$ be a solution of the free Klein-Gordon equation. Let us write

$$\phi(\vec{r},t) = \psi(\vec{r},t)e^{-imc^2t/\hbar}$$

Under what conditions will $\psi(\vec{r}, t)$ be a solution of the non-relativistic Schrodinger equation? Interpret your condition physically when ϕ is given by a plane-wave solution.

20.8.16 Matrix Representation of Dirac Matrices

The Dirac matrices must satisfy the anti-commutator relationships:

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}$$
, $\{\alpha_i, \beta\} = 0$ with $\beta^2 = 1$

- (1) Show that the α_i , β are Hermitian, traceless matrices with eigenvalues ± 1 and even dimensionality.
- (2) Show that, as long as the mass term mis not zero and the matrix β is needed, there is no 2 × 2 set of matrices that satisfy all the above relationships. Hence the Dirtac matrices must be of dimension 4 or higher. First show that the set of matrices $\{I, \vec{\sigma}\}$ can be used to express any 2 × 2

matrix, i.e., the coefficients c_0 , c_i always exist such that any 2×2 matrix can be written as:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = c_0 I + c_i \sigma_i$$

Having shown this, you can pick an intelligent choice for the α_i in terms of the Pauli matrices, for example $\alpha_i = \sigma_i$ which automatically obeys $\{\alpha_i, \alpha_j\} = 2\delta_{ij}$, and express β in terms of $\{I, \vec{\sigma}\}$ using the relation above. Show then that there is no $2 \times 2 \beta$ matrix that satisfies $\{\alpha_i, \beta\} = 0$.

20.8.17 Weyl Representation

(1) Show that the Weyl matrices:

$$\vec{\alpha} = \begin{pmatrix} -\vec{\sigma} & 0\\ 0 & \vec{\sigma} \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} 0 & I\\ I & 0 \end{pmatrix}$$

satisfy all the Dirac conditions of Problem 20.16. Hence, they form just another representation of the Dirac matrices, the Weyl representation, which is different than the standard Pauli-Dirac representation.

(2) Show that the Dirac matrices in the Weyl representation are

$$\vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix} \quad , \quad \gamma^0 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$$

- (3) Show that in the Weyl representation $\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} -I & 0\\ 0 & I \end{pmatrix}$
- (4) Solve the Dirac equation $[\vec{\alpha} \cdot \vec{p} + \beta m]\Psi = E\Psi$ in the particle rest frame using the Weyl representation.
- (5) Compute the result of the chirality operators

$$\frac{1 \pm \gamma_5}{2}$$

when they are acting on the Dirac solutions in the Weyl representation.

20.8.18 Total Angular Momentum

Use the Dirac Hamiltonian in the standard Pauli-Dirac representation

$$H = \vec{\alpha} \cdot \vec{p} + \beta m$$

to compute $[H, \hat{L}]$ and $[H, \hat{\Sigma}]$ and show that they are zero. Use the results to show that:

$$[H, \hat{L} + \hat{\Sigma}/2] = 0$$

where the components of the angular momentum operator are given by:

$$\hat{L}_i = \varepsilon_{ijk} \hat{x}_j \hat{p}_k$$

and the components of the spin operator are given by:

$$\hat{\Sigma}_i = \begin{pmatrix} \sigma^i & 0\\ 0 & \sigma^i \end{pmatrix}$$

Recall that the Pauli matrices satisfy $\sigma^i \sigma^j = \delta^{ij} + i \varepsilon^{ijk} \sigma^k$.

20.8.19 Dirac Free Particle

The Dirac equation for a free particle is

$$i\hbar\frac{\partial\left|\psi\right\rangle}{\partial t}=\left(c\alpha_{x}p_{x}+c\alpha_{y}p_{y}+c\alpha_{z}p_{z}+\beta mc^{2}\right)\left|\psi\right\rangle$$

Find all solutions and discuss their meaning. Using the identity

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + i\vec{\sigma} \cdot (\vec{A} \times \vec{B})$$

will be useful.

Chapter 21

Interacting Fields and Feynman Diagrams

21.1 Relativistic Quantum Mechanics of Free Particles

21.1.1 Hilbert Space

In a quantum mechanical description, the state of a free, spinless particle is completely specified by its three-momentum since its energy follows from the energy-momentum relation. This is called the momentum-space description. A particle with well-defined momentum (and energy) is described by a plane wave and $E = h\nu$.

In addition, we will assume superposition is valid for quantum mechanical states. Finally, we will assume that only particles of one type exist. Let us now implement these statements mathematically. We will set $\hbar = 1$ and c = 1 from now on.

We assume the existence of an infinite dimensional Hilbert space and that for every possible physical state there is a vector in the space. We choose the vectors corresponding to a particle with momentum \vec{p} , $|\vec{p}\rangle$ as basis vectors of length 1. The Hilbert space basis is thus:

- $|0\rangle$ corresponding to the vacuum
- $|\vec{p}_1\rangle$ corresponding to a particle of momentum \vec{p}_1
- $|\vec{p}_2\rangle$ corresponding to a particle of momentum \vec{p}_2
-

 $|\vec{p}_1,\vec{q}_1\rangle$ corresponding to two particles one of momentum \vec{p}_1 , the other \vec{q}_1 and so on

The basis vectors are orthonormal, i.e.,

$$\langle \vec{p} \mid \vec{q} \rangle = \delta_{\vec{p}\vec{q}} \tag{21.1}$$

Since the range of momenta is infinite the subspace of the single particles is infinite dimensional.

For mathematical convenience, we will assume that the universe is a cube with volume V and we allow only those wave functions whose value on the boundary is the same as the value on the opposite boundary (called periodic boundary conditions). This means that we are working with a infinite, but denumerable, dimensional Hilbert space, where the momenta are restricted to the discrete values (L = length of a side of the cube) given by

$$p_1 = \pm \frac{2\pi n_1}{L} , \ p_2 = \pm \frac{2\pi n_2}{L} , \ p_3 = \pm \frac{2\pi n_3}{L} \quad n_1 , n_2 , \ n_3 = 0, 1, 2, \dots$$
(21.2)

At the end of any calculations, we take the limit $V \to \infty$ thus returning to the true continuous case. In the limit any sum over momenta becomes an integral by the rule

$$\sum_{\vec{p}} \rightarrow \frac{V}{(2\pi)^3} \int d^3p \tag{21.3}$$

The factor

$$\frac{V}{(2\pi)^3}$$
 (21.4)

arises because in a little box d^3p there will be that many possible states(possible momentum values in phase space).

T 7

In addition we have

$$\lim_{V \to \infty} \frac{V}{(2\pi)^3} \delta_{\vec{p}_i \vec{p}_j} = \delta^{(3)} (\vec{p}_i - \vec{p}_j)$$
(21.5)

What we are doing here is of course quite horrible for any relativistic theory. We are violating Lorentz invariance.

A cubical box of volume V is not Lorentz invariant. However, we assume that our final results will be Lorentz invariant in the limit of infinite V. This plague, having to abandon Lorentz invariance in order to define the formalism, is common to all approaches to quantum field theory(QFT). One always needs some kind of grid to work on. The final results, the Feynman rules, do not suffer, however, from the breaking of Lorentz invariance.

Since quantum mechanics will form the basis of our derivation of QFT and the Feynman rules, a review(from a different point of view) of the basic concepts is in order.

The wave function of a non-relativistic particle is

$$\psi(x,t) = \frac{1}{\sqrt{V}} e^{i(\vec{p}\cdot\vec{x} - E_p t)}$$
(21.6)
where

$$E_p = \text{non - relativistic kinetic energy} = \frac{1}{2}m\vec{v}^2 = \frac{\vec{p}^2}{2m}$$
 (21.7)

and the normalization is such that the total probability (integrating over the whole universe of volume V is 1. This wave function describes one particle in the universe and it is a solution of *Schrödinger's equation*

$$\frac{1}{2m}\nabla^2\psi = -i\frac{\partial\psi}{\partial t} \tag{21.8}$$

The relativistic generalization of the wave function is simple:

$$\psi(x) = \frac{1}{\sqrt{V}} e^{i(px)} = \frac{1}{\sqrt{V}} e^{i(\vec{p}\cdot\vec{x}-Et)}$$
(21.9)

where

$$E = \text{ relativistic kinetic energy } = \sqrt{\vec{p}^2 + m^2}$$
 (21.10)

and the wave function is now a solution of the Klein-Gordon equation:

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - m^2\right)\psi(x) = \left(E^2 - p^2 - m^2\right)\psi(x) = 0$$
(21.11)

In making the relativistic transition, the definition of probability needs some revision. In the non-relativistic theory the probability density to find a particle at some point x within a small box d^3x is given by

$$|\psi(x)|^2 d^3x \tag{21.12}$$

where the integral of this expression over the whole volume must be equal to 1. However, since the volume is not a Lorentz invariant, we cannot maintain this definition of probability density. Probability density does not need to be a Lorentz invariant, only the total probability must be Lorentz invariant (and equal to 1). This is very much like electric charge. In fact, if we assume that like electric charge density and current, the probability density (P_0) and its associated probability current ($\vec{P} = (P_1, P_2, P_3)$) satisfies a conservation (continuity) equation, then we have (pushing on the analogy)

$$\partial_{\mu}P_{\mu} = 0 \leftrightarrow \partial_{\mu}j_{\mu} = 0 \tag{21.13}$$

It then follows that the total probability (like total electric charge) is given by

$$P = \int d^3x P_0(x)$$
 (21.14)

In the same manner that we can prove total charge is constant, we can then prove that P is a constant or $\partial P/\partial t = 0$ (assumes that P is zero on the boundary of a surface integral).

For consistency, we must have that the charge density is proportional to probability density. The formal definition of P_{μ} is

$$P_{\mu}(x) = i \frac{\partial \psi^{*}(x)}{\partial x_{\mu}} \psi(x) - i \psi^{*}(x) \frac{\partial \psi(x)}{\partial x_{\mu}}$$
(21.15)

In this case, since, in the low energy limit, $E \approx m$ and $P_0 \approx 2m\psi^*\psi$, by normalizing ψ as follows

$$\psi(x) = \frac{1}{\sqrt{2Vp_0}} e^{i(px)}$$
(21.16)

we have normalization equal to 1 when integrating P_0 over the whole volume V.

Since particles do have a location in space, we must now consider states that are not pure plane waves. A particle that we know is precisely at the point \vec{x} at time x_0 (we will take $x_0 = 0$) is described at time 0 by a δ -function

$$\psi(\vec{x},0) = C\delta^{(3)}(\vec{x}) \tag{21.17}$$

where C is a normalization constant. This can be seen as a superposition of *pure momentum states*:

$$\psi(\vec{x},0) = \frac{C}{(2\pi)^3} \int d^3p \, e^{i\vec{p}\cdot\vec{x}}$$
(21.18)

which we generalize to

$$\psi(\vec{x},t) = \psi(x) = \frac{C}{(2\pi)^3} \int d^3p \, e^{i(px)}$$
(21.19)

where

$$px = p_0 x_0 - \vec{p} \cdot \vec{x} = Et - \vec{p} \cdot \vec{x} , \quad E^2 = \vec{p}^2 + m^2$$
(21.20)

so that it satisfies the Klein-Gordon equation.

If the location is not a δ -function but more smeared out, then we have, in general:

$$\psi(x) = \frac{C}{(2\pi)^3} \int d^3p f(p) e^{i(px)} , \ p_0^2 = \vec{p}^2 + m^2$$
(21.21)

For example, if f(p) = 1, we have a δ -function in space and if $f(p) = \delta^{(3)}(\vec{p} - \vec{q})$ we have a state with sharply defined momentum \vec{q} . Therefore, the vector in Hilbert space that corresponds to a sharply defined location at some time will be a superposition of sharp momentum states with equal weight:

$$|\vec{x}, x_0\rangle = \sum_{\vec{p}} C e^{i(px)} |\vec{p}\rangle$$
(21.22)

What happens to a state in Hilbert space when we apply a Lorentz transformation? The Lorentz transformation L directly transforms any momentum p into p' where Lp = p'. It is a 4×4 matrix in a 4-dimensional space. In Hilbert space vectors, it must transform the arguments of all of the different ket vectors, i.e.,

$$\begin{aligned} & |\vec{p}_1\rangle \rightarrow |\vec{p}_1'\rangle \\ & |\vec{p}_2\rangle \rightarrow |\vec{p}_2'\rangle \\ & |\vec{p}_1, \vec{q}_1\rangle \rightarrow |\vec{p}_1', \vec{q}_1'\rangle \end{aligned}$$

and so on.

This is an $\infty \times \infty$ transformation matrix. Luckily we never need to write it down, but only know what it does. Let us consider a simpler example, namely, the behavior under translations. Under a space-time translation $b = (b_0, \vec{x})$ a particle sharply located at place \vec{x} , time x_0 , will become a particle sharply located at place $\vec{x} + \vec{b}$ and time $x_0 + b_0$. Thus

$$T(b) : |x\rangle \to |x+b\rangle \tag{21.23}$$

and

$$\sum_{\vec{p}} e^{i(px)} \left| \vec{p} \right\rangle \to \sum_{\vec{p}} e^{i(px) + i(pb)} \left| \vec{p} \right\rangle \tag{21.24}$$

Therefore, under a translation the state $|\vec{p}\rangle$ goes over into the state $e^{ipb} |\vec{p}\rangle$. This shows explicitly how the transformation of the vectors in Hilbert space differs from what happens in ordinary space. The vector *just gets a phase factor*, that is, *it stays normalized and represents, physically speaking, the same state.*

General Rule

To every Lorentz transformation there corresponds a transformation in Hilbert space.

Our physics must be unique, so we insist that we have a 1-1 correspondence. This means that labeling the Hilbert space transformation by X,

$$L_1 \rightarrow X_1$$

$$L_2 \rightarrow X_2$$

$$L_3 = L_1 L_2 \rightarrow X_1 X_2 = X_3$$

which implies that the transformations in Hilbert space are a *representation of* the Lorentz group.

Matrices in Hilbert Space

In order to describe physical processes we must introduce operators (matrices) in the Hilbert space. A typical process, for example electrons scattering off a proton, involves different states from the point of view of Hilbert space. Thus initially we may have an electron of momentum \vec{p} and a proton of momentum \vec{k} ,

which corresponds the basis vector $|\vec{p}, \vec{k}\rangle$ in Hilbert space and the final state may then contain an electron and proton of momenta \vec{p}' and a proton of momentum \vec{k}' , corresponding to the vector $|\vec{p}', \vec{k}'\rangle$ in Hilbert space. It seems like we might think of this as if the physical system corresponds to a vector in Hilbert space that rotates as a function of time from $|\vec{p}, \vec{k}\rangle$ to $|\vec{p}', \vec{k}'\rangle$.

We cannot, however, describe things in this way. The reason is that scattering clearly involves interaction between particles, and we have set up our Hilbert space for free particles only. We must rethink our procedures if we want to introduce interactions.

Right now it suffices to say that physical quantities will correspond to the elements of a certain matrix defined in Hilbert space. What we need is basic building blocks, in some sense matrices like the Pauli spin matrices that can be used to describe the full set of 2×2 matrices. The matrices that we need will fulfill certain basic requirements, in particular the requirement of locality. This is the requirement that physical processes cannot influence each other if they are outside each other's light cone, i.e., if speeds larger than that of light are needed to connect the events.

This we hope will be achieved by insisting that the operator (matrix) describing a process at the space-time point x will *commute* with a similar operator for the space-time point y if x and y are *outside each other's light cone*.

Locality is a touchy point of quantum theory, and to a large extent it remains, in its formulation, an article of faith. There is however, at this time, no reason to suspect anything wrong with the procedure adopted above.

To explain what we are going to do let us first consider three-dimensional space.

What would be the most elementary building blocks that can be used to build up any 3×3 matrix? We can do this with two matrices:

$$a = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \quad , \quad \bar{a} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$
(21.25)

This can be seen by working out the various products involving a and \bar{a} and showing that any 3×3 matrix can be obtained as a linear combination of these matrices and associated products. The factor $\sqrt{2}$ was introduced for reasons that will become transparent later.

We now turn to Hilbert space.

The above example can be used for the subspace referring to a definite momen-

tum \vec{p} . A matrix *a* as above can be constructed in the subspace of states:

$$|0\rangle = \begin{pmatrix} 1\\0\\0 \end{pmatrix} , \quad |\vec{p}\rangle = \begin{pmatrix} 0\\1\\0 \end{pmatrix} , \quad |\vec{p},\vec{p},\rangle = \begin{pmatrix} 0\\0\\1 \end{pmatrix}$$
(21.26)

These matrices represent a universe with n particles all with the same momentum \vec{p} where $0 \le n \le 2$ as can be seen from the relations

$$\begin{split} a & |0\rangle = 0 \ , \ a & |\vec{p}\rangle = |0\rangle \ , \ a & |\vec{p}, \vec{p}\rangle = \sqrt{2} & |\vec{p}\rangle \\ \bar{a} & |0\rangle = & |\vec{p}\rangle \ , \ \bar{a} & |\vec{p}\rangle = \sqrt{2} & |\vec{p}, \vec{p}\rangle \ , \ \bar{a} & |\vec{p}, \vec{p}\rangle = 0 \\ \bar{a}a & |0\rangle = 0 \ , \ \bar{a}a & |\vec{p}\rangle = 1 & |\vec{p}\rangle \ , \ \bar{a}a & |\vec{p}, \vec{p}\rangle = 2 & |\vec{p}, \vec{p}\rangle \end{split}$$

We may extend the example to more dimensions. In a large dimensional space we still can do everything with two matrices a and \bar{a} with

The above example can be used for the subspace referring to a definite momentum \vec{p} . A matrix a as above can be constructed in the subspace of states

$$|0\rangle , |\vec{p}\rangle , |\vec{p},\vec{p},\rangle , etc$$
 (21.28)

The matrix a when applied to a state vector with n particles of momentum \vec{p} then gives the vector for a state with n-1 particles of momentum \vec{p} with a factor \sqrt{n} as we saw in the special case $0 \le n \le 2$ above.

Examples

Consider

$$a |\vec{p}, \vec{p}, \vec{p}\rangle = \sqrt{3} |\vec{p}, \vec{p}\rangle , \quad a |0\rangle = 0$$
 (21.29)

This particular matrix operating in the \vec{p} subspace will be denoted by $a(\vec{p})$. Similarly, we will have matrices for any other subspace, and we then have an infinite set of matrices $a(\vec{p})$ and $a^+(\vec{p})$ (with $a^+ = a^{*T}$ which is the same as a^T since a is real here).

Having done this, we do not need to introduce new matrices for that part of Hilbert space where we have particles of different momenta, such as the state $|\vec{p}, \vec{p}, \vec{q}, \vec{q}, \vec{q}\rangle$ with $\vec{p} \neq \vec{q}$. The matrices $a(\vec{p})$ and $a(\vec{q})$ will by definition act on these states as if the other particles are not there. Thus (with $\vec{p} \neq \vec{q}$):

$$\begin{aligned} a(\vec{p}) \left| \vec{q}, \vec{q}, \vec{q}, \vec{q} \right\rangle &= 0 \\ a(\vec{p}) \left| \vec{p}, \vec{p}, \vec{q}, \vec{q} \right\rangle &= \sqrt{2} \left| \vec{p}, \vec{q}, \vec{q}, \vec{q} \right\rangle \\ a(\vec{q}) \left| \vec{p}, \vec{p}, \vec{q}, \vec{q} \right\rangle &= \sqrt{3} \left| \vec{p}, \vec{p}, \vec{q}, \vec{q} \right\rangle \end{aligned}$$

and so on.

We now have a set of matrices $a(\vec{p})$ and $a^+(\vec{p})$, called *annihilation and creation* operators respectively, defined over the whole Hilbert space, that can be used to build up any other matrix(operator). Note that by construction $a(\vec{p})a(\vec{q}) =$ $a(\vec{q})a(\vec{p})$ if $\vec{p} \neq \vec{q}$ and of course also if $\vec{p} = \vec{q}$. They do not interfere with each other.

The matrix

$$H = \sum_{\vec{p}} p_0 a^+(\vec{p}) a(\vec{p}) \quad , \quad p_0 = \sqrt{\vec{p}^2 + m^2}$$
(21.30)

is diagonal (as seen from the relations in the above example) and it is the energy operator, that is:

$$H\left|\alpha\right\rangle = E_{\alpha}\left|\alpha\right\rangle \tag{21.31}$$

where E_{α} is the total energy of the state $|\alpha\rangle$. Here α may be any number of particles of any momentum. Explicitly, we have

$$\begin{split} H \left| 0 \right\rangle &= 0 \quad , \quad H \left| \vec{q} \right\rangle = q_0 \left| \vec{q} \right\rangle \quad , \\ H \left| \vec{p}, \vec{p} \right\rangle &= 2 p_0 \left| \vec{p}, \vec{p} \right\rangle \quad , \quad H \left| \vec{p}, \vec{q} \right\rangle = \left(p_0 + q_0 \right) \left| \vec{p}, \vec{q} \right\rangle \end{aligned}$$

and so on.

21.1.2 Fields

The Fourier transforms of the matrices a and a^+ are called *fields*. To be precise we have the field A(x):

$$A(x) = \sum_{\vec{p}} \frac{1}{\sqrt{2Vp_0}} a(\vec{p}) e^{-ipx}$$
(21.32)

Similarly

$$A^{+}(x) = \sum_{\vec{p}} \frac{1}{\sqrt{2Vp_0}} a^{+}(\vec{p}) e^{-ipx}$$
(21.33)

Notice that A(x) is no longer a real matrix due to the complex factors exp(-ipx). The matrices A(x) and $A^+(x)$ can be taken as basic building blocks also since a can be recovered from A. For example, $a(\vec{q})$ can be obtained from A(x) by another Fourier transformation:

$$\int d^3x \, e^{iqx} A(x) = \frac{1}{\sqrt{2Vp_0}} a(\vec{q}) \tag{21.34}$$

The Hermitian combination

$$\varphi(x) = A(x) + A^{+}(x)$$
 (21.35)

is called the *field* corresponding to the particles considered. This field has a number of properties that make it very useful for the construction of physical quantities. The main property is that it is local.

The commutator

$$[\varphi(x),\varphi(y)] = \varphi(x)\varphi(y) - \varphi(y)\varphi(x)$$
(21.36)

is zero if x and y are outside of each other's light cone. To see this we compute things step by step:

$$[A(x), A(y)] = 0 ext{ This follows because } a(\vec{p})a(\vec{q}) = a(\vec{q})a(\vec{p}) \\ [A^+(x), A^+(y)] = 0 ext{ This follows because } a^+(\vec{p})a^+(\vec{q}) = a^+(\vec{q})a^+(\vec{p}) \\ [A(x), A^+(y)] = \sum_{\vec{p}} \frac{1}{2Vp_0} e^{-ip(x-y)} ext{ (21.37)}$$

$$[A^{+}(x), A(y)] = -\sum_{\vec{p}} \frac{1}{2Vp_0} e^{ip(x-y)}$$
(21.38)

These last two results follow from the equations

$$[a(\vec{p}), a^{+}(\vec{q})] = \delta_{\vec{p}\vec{q}} = -[a^{+}(\vec{p}), a(\vec{q})]$$
(21.39)

Altogether we find:

$$[\varphi(x),\varphi(y)] = \sum_{\vec{p}} \frac{1}{2Vp_0} \left(e^{ip(x-y)} - e^{-ip(x-y)} \right)$$
(21.40)

We now show that the right hand side is zero if x and y are outside each other's light cone. First we take the continuum limit, $V \rightarrow \infty$:

$$\sum_{\vec{p}} \to \int d^3 p \frac{V}{(2\pi)^3}$$

Calling the right hand side of the above commutator the function $\Delta_c(x-y)$ we have,

$$\Delta_c(x-y) = \frac{1}{(2\pi)^3} \int d^3p \frac{1}{2p_0} \left(e^{ip(x-y)} - e^{-ip(x-y)} \right)$$
(21.41)

To prove that this is zero if the four vector z = x - y is outside the light cone (which means (zz > 0) we proceed in two steps. First we will show that Δ_c is Lorentz invariant. Then we will show that $\Delta_c(z)$ is zero for any z with $z_0 = 0$ by a Lorentz transformation (that leaves Δ_c unchanged) we will have proven the required result. The argument is illustrated in Figure 21.1 below.



Figure 21.1: Light Cone Arguments

If the function is zero at the location of the cross it is zero in the whole shell(formed from curve shown) going through that point, because all the points in the shell can be obtained from the cross point by means of a Lorentz transformation, and the function is Lorentz invariant. If the function is zero along the whole horizontal axis (the equal time line) then the function is zero everywhere outside the light cone.

To show the Lorentz invariance we first rewrite the three-dimensional integral as a four-dimensional integral. This may be done as follows.

Note that in the above $p_0 = \sqrt{\vec{p}^2 + m^2}$. We write

$$\frac{1}{2p_0} = \int_{-q}^{q} d\xi \delta(\xi^2 - \vec{p}^2 - m^2)\theta(\xi)$$
(21.42)

where

$$\theta(\xi) = \begin{cases} 1 & \text{if } \xi > 0 \\ 0 & \text{if } \xi < 0 \end{cases}$$
(21.43)

Indeed, the only points contributing to the integral are

$$\xi = \pm \sqrt{\vec{p}^2 + m^2} \tag{21.44}$$

We may write

$$\delta(\xi^2 - \vec{p}^2 - m^2) = \delta((\xi - \sqrt{\vec{p}^2 + m^2})(\xi + \sqrt{\vec{p}^2 + m^2}))$$
(21.45)

Now

$$\delta(ab) = \frac{1}{|a|}\delta(b) + \frac{1}{|b|}\delta(a)$$
(21.46)

Furthermore, the solution $\xi = -\sqrt{\vec{p}^2 + m^2}$ will not give anything because the θ -function restricts us to positive values for ξ . Thus, we get

$$\frac{1}{2p_0} = \int_{-q}^{q} d\xi \frac{1}{\xi + \sqrt{\vec{p}^2 + m^2}} \delta(\xi - \sqrt{\vec{p}^2 + m^2}) \theta(\xi) = \frac{1}{2\sqrt{\vec{p}^2 + m^2}}$$
(21.47)

which is in agreement with what we stated above.

Although it might cause some confusion we are going to use for ξ the name p_0 , and the above result is

$$\frac{1}{2p_0} = \int_{-q}^{q} dp_0 \delta(p_0^2 - \vec{p}^2 - m^2) \theta(p_0)$$
(21.48)

Using this result, the function Δ_c becomes

$$\Delta_{c}(z) = \frac{1}{(2\pi)^{3}} \int d^{3}p \int_{-q}^{q} dp_{0} \delta(p_{0}^{2} - \vec{p}^{2} - m^{2}) \theta(p_{0}) \left(e^{ip(z)} - e^{-ip(z)}\right)$$
$$= \frac{1}{(2\pi)^{3}} \int d^{4}p \delta(p^{2} - m^{2}) \left(e^{ipz} - e^{-ipz}\right) \theta(p_{0})$$
(21.49)

where we have used $\delta(a) = \delta(-a)$.

We now show that this integral is Lorentz invariant. Thus, we will let z = Lz', where L is some Lorentz transformation, and we will show that

$$\Delta_c(z) = \Delta_c(z') \tag{21.50}$$

We have

$$\Delta_c(z) = \Delta_c(Lz') = \frac{1}{(2\pi)^3} \int d^4p \delta(p^2 - m^2) \left(e^{ipLz'} - e^{-ipLz'} \right) \theta(p_0) \quad (21.51)$$

Now introduce four new variables q_1, q_2, q_3, q_4 related to the p by p = Lq. This is as if we did a Lorentz transformation on p, but it is really a change of integration variables. The integration volume element d^4p becomes d^4q times the Jacobian of transformation

$$d^4p = \det(L)d^4q \tag{21.52}$$

Since det(L) = 1 that gives no change. Furthermore:

$$(p, Lz') = (Lq, Lz') = (q, z')$$

 $p^2 = (p, p) = (Lq, Lq) = (q, q) = q^2$

Finally, what happens with $\theta(p_0)$? This is more subtle and requires a detailed investigation of the action of a Lorentz transformation on the vector p. This vector is restricted to values inside the upper light cone, because we must have

 $p^2 = m^2$ (*p* is said to be on the mass-shell) and the θ -function restricts us to the upper light cone. Since any four-vector in the upper light cone transforms into another vector in the upper light cone, *q* will also be in the upper light cone. Therefore, $\theta(q_0)$ will also be non-zero if $\theta(p_0)$ was nonzero and zero if $\theta(p_0)$ was zero. In other words, $\theta(p_0) = \theta(q_0)$ if p = Lq, but for this the δ -function is crucial, because otherwise there would not be the restriction to the upper light cone. The result of all this is:

$$\Delta_c(z) = \frac{1}{(2\pi)^3} \int d^4q \delta(q^2 - m^2) \left(e^{iqz'} - e^{-iqz'} \right) \theta(q_0) = \Delta_c(z')$$
(21.53)

The last step follows since this differs from the original expression only by a different notation for the integration variables.

Now step 2. Let us suppose $z_0 = 0$. Then

$$\Delta_c(z)_{z_0=0} = \frac{1}{(2\pi)^3} \int d^4q \delta(q^2 - m^2) \left(e^{iqz'} - e^{-iqz'} \right) \theta(q_0)$$
(21.54)

The $\theta\delta$ actor restricts the q_0 integration but not the \vec{q} integration. The \vec{q} integral goes from $-\infty$ to $+\infty$ for every component. Therefore

$$\int d^3q f(\vec{q}) = \int d^3q f(-\vec{q}) \tag{21.55}$$

and we see that the two terms cancel and thus

$$\Delta_c(z)_{z_0=0} = 0 \tag{21.56}$$

This concludes the proof.

Another important property of the field φ is that it obeys the Klein-Gordon equation. The complete expression for the field $\varphi(x)$ is:

$$\varphi(x) = \sum_{\vec{p}} \frac{1}{\sqrt{2Vp_0}} (a(\vec{p})e^{-ipx} + a^+(\vec{p})e^{ipx}) \quad , \quad p_0 = \sqrt{\vec{p}^2 + m^2}$$
(21.57)

It is easy to see that

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - m^2\right)\varphi(x) = 0$$
(21.58)

due to the mass-shell relation for p_0 . Finally, operating with $\varphi(x)$ on the vacuum state we obtain the state for a particle located at the point x at time $x_0 = 0$ we have

$$\varphi(x)|0\rangle = \sum_{\vec{p}} \frac{1}{\sqrt{2Vp_0}} (a(\vec{p})e^{-ipx} + a^+(\vec{p})e^{ipx})|0\rangle = \sum_{\vec{p}} \frac{1}{\sqrt{2Vp_0}} e^{ipx}|p\rangle \quad (21.59)$$

We can also derive commutation rules for equal times.

$$[\varphi(x),\varphi(y)]_{x_0=y_0} = \Delta_c(z)_{z_0=0} = 0 \quad , \quad z = x - y \tag{21.60}$$

$$\left[\frac{\partial\varphi(x)}{\partial x_0},\varphi(y)\right]_{x_0=y_0} = i\left(\frac{\partial\Delta_c(z)}{\partial x_0}\right)_{z_0=0} = -i\delta^{(3)}(\vec{x}-\vec{y})$$
(21.61)

21.1.3 Structure of Hilbert Space

The connection between vectors in Hilbert space and measurements in quantum mechanics is through probability. Physical states correspond to vectors(of unit length) in Hilbert space, where length is defined by the usual scalar-product in complex space. If a vector $|\xi\rangle$ has the components $\xi_1, \xi_2, ...$, that is

$$|\xi\rangle = \xi_1 |1\rangle + \xi_2 |2\rangle + \dots$$
 (21.62)

where $|1\rangle, |2\rangle, ...,$ etc, represent the first, second, etc, basis vectors. Then the scalar-product of $|\xi\rangle$ with itself is given by

$$\langle \xi \mid \xi \rangle = \xi_1^* \xi_1 + \xi_2^* \xi_2 + \dots$$
(21.63)

Similarly,

$$\langle \eta | \xi \rangle = \eta_1^* \xi_1 + \eta_2^* \xi_2 + \dots = \sum_i \eta_i^* \xi_i$$
 (21.64)

The connection with physical measurements is now as follows. Suppose we have a vector $|c\rangle$ corresponding to some physical system. Now, let there be two other mutually orthogonal vectors $|a\rangle$ and $|b\rangle$, also corresponding to physical systems. Suppose now $|c\rangle = \alpha |a\rangle + \beta |b\rangle$. Remember that $|a\rangle$, $|b\rangle$ and $|c\rangle$ must all be of unit length, because they represent physical states.

Now, if the system is in the state described by $|c\rangle$ and one tries to measure whether the system is **in** state $|a\rangle$ or $|b\rangle$ one will find:

probability to find system in state
$$|a\rangle = |\alpha|^2$$
 (21.65)

probability to find system in state $|b\rangle = |\beta|^2$ (21.66)

Here in means that the system is measured to have the same properties as state a or state b.

More generally, if a system is in a state $|c\rangle$, then the probability to observe the state $|a\rangle$ is given by

$$\left|\left\langle a \mid c\right\rangle\right|^2 \tag{21.67}$$

This is the *fundamental connection* between Hilbert space and physical measurements. Since $\langle c | c \rangle = 1$ we must have

$$|\alpha|^2 + |\beta|^2 = 1 \tag{21.68}$$

The two probabilities add up to 1, as should, of course, be the case.

There is some potential trouble here in connection with Lorentz invariance, quite different from the trouble arising from dealing with a finite volume. As noted before, states in Hilbert space are generally not invariant under Lorentz transformations, but they transform according to some representation of these Lorentz transformations. The trouble now is that we certainly want probabilities to be invariant under Lorentz transformations, in other words, the above defined scalar-product must be invariant.

In addition, since the scalar-products are no longer necessarily positive, we must then insist that states with negative probability are unphysical.

By itself this is not new: even in ordinary space there are restrictions, and momenta of particles are physical only if their scalar-product with themselves is positive (corresponding to real mass). Particles with momenta such that (pp)is negative have not been seen.

So, much the same as in ordinary space where some domains seem to be excluded for physics, the same might happen in Hilbert space. In Hilbert space, we would be truly in difficulty if we had to allow for physical systems with negative probability. No consistent theory can then be constructed, because probability is positive by its very definition.

For scalar or pseudoscalar particles there is not yet any problem, the transformations in Hilbert space are rather trivial (as for example the Hilbert space vector $|\vec{p}\rangle$ transforming to the vector $|\vec{q}\rangle$ where \vec{q} is the Lorentz transform of \vec{p} . In dealing with particles with spin, such as electrons and photons, the transformation of the states in Hilbert space becomes more complicated and we leave that for a more advanced text.

21.2 Interacting Fields - Part 1

21.2.1 Physical System

We will now discuss systems of interacting particles.

We use the Lehmann-Symanzik-Zimmermann formalism, and Kallen's method to derive the S-matrix from the equations of motion.

For definiteness, we assume the existence of two kinds of particles called π and σ . Both are spinless, since including that complication is not needed to understand the derivation of Feynman rules. We assume masses M and m for the π and σ respectively. This model is a simplified version of electrodynamics of electrons and photons. The π will play the role of the photon.

To begin we will focus on a specific problem, namely $\pi\pi$ scattering. The physical process is shown in Figure 21.2 below.

Two pions with momenta p and q (with $p^2 = q^2 = M^2$) meet and scatter, and we are interested in the probability that a final configuration of two pions with momenta p' and q' (with $p'^2 = q'^2 = M^2$) is produced. This probability, when



Figure 21.2: $\pi\pi$ scattering

multiplied with the appropriate flux factors, will be the *differential cross section* for this process.

21.2.2 Hilbert Space

This aspect needs very careful consideration. A vector in Hilbert space represents a physical state.

What is a physical state?

A physical state is simply a possible physical system, with particles moving here and there, with collisions, with dogs chasing cats, with people living and dying, with all kinds of things happening.

Often people make the mistake of identifying a physical state with the system at a given moment, one picture from a movie, but that is not what we call the physical state. The system at some moment may be seen as a boundary condition, that is, if one knows the whole system at some moment, and one knows the laws of nature, then in principle we can deduce the rest!

Thus a physical state may be characterized by the system at a definite moment, but the state itself refers to the whole world including its progress in time.

Conveniently, especially for scattering processes one may use the time points $\pm\infty$. Thus the above process corresponds to a vector in Hilbert space, and we can denote that vector by

$$|p,q\rangle_{in} \tag{21.69}$$

By this we mean: that physical system that has two pions of momenta p and q at time $t = -\infty$ (the *in* configuration). It must be understood that $|p,q\rangle_{in}$ contains everything, including how the system looks at other times. For example, we could define the state $|p,q\rangle_0$ as that physical system which has at time t = 0 exactly two pions of momenta p and q. The above described state, $|p,q\rangle_{in}$, has two such pions at $t = -\infty$, but it may well be that they scatter before t = 0, and, thus, the probability that we have still two pions with that same momentum at t = 0 is smaller than one.

The above discussion leads up to the following identification.

Let $|p,q\rangle_{in}$ and $|p,q\rangle_0$ be the systems as described above. They are different systems. Let the system be in the state $|p,q\rangle_{in}$ (two pions at $t = -\infty$). The probability of having two pions with momenta p and q at t = 0 is the square of the absolute value of the scalar-product between the states:

$$\left|_{0}\left\langle p,q \mid p,q\right\rangle_{in}\right|^{2} \tag{21.70}$$

If some collision took place before t = 0 we may actually still have two pions but with different momenta, say k and r. A state with two pions with momenta kand r at time t = 0 is denoted by $|k, r\rangle_0$. If the system is in the state $|p, q\rangle_{in}$ then the probability of observing two pions of momenta k and r at t = 0 is given by:

$$\left|_{0}\left\langle k,r \mid p,q\right\rangle_{in}\right|^{2} \tag{21.71}$$

Thus the state $|p,q\rangle_{in}$ when viewed at time $t = -\infty$ contains two pions of momenta p and q, but if we look to it at time t = 0 we see with some probability two pions that may or may not have the momenta p and q. More generally, new particles may be produced in a collision, so we may also see three, four, etc. pion configurations. For example,

$$\left|_{0}\left\langle k,r,s\mid p,q\right\rangle_{in}\right|^{2}\tag{21.72}$$

gives the probability of observing three pions of momenta k, r and s at time t = 0 if we know that the system is in a state characterized by the fact that at time $t = -\infty$ there were two pions of momenta p and q.

Magnitude of Hilbert Space

It follows from the above that we can have as many states in Hilbert space as possible systems at $t = -\infty$.

We now assume the following *asymptotic condition*: if particles are sufficiently far apart in space they do not interact and behave as free particles. If we go sufficiently far back in time, particles will be separated. Therefore, we may assume that the possible systems at $t = -\infty$ are precisely the systems of non-interacting particles.

Thus the Hilbert space of interacting systems is by this assumption equally as large as the Hilbert space of free particles.

Clearly, we will have to modify this if we want to consider stable bound states. No matter how far back we go in time, the electron and proton in a hydrogen atom do not separate. To describe such systems properly we must enlarge Hilbert space and allow states containing hydrogen atoms. Of course, such atoms again can just be considered as a new kind of particle, and the Hilbert space becomes then effectively the free Hilbert space of three (in this case) particles (electrons, protons and hydrogen atoms). We will consider, however, only simple particle states.

Now that we are clear about the meaning of states and their representation in Hilbert space we can proceed and postulate equations that will describe particles in interactions. Experiment must then decide which equations describe nature. Of course, whatever we postulate, it will be within the framework of Lorentz invariant quantum mechanics. Only a limited degree of freedom is left.

U-matrix, S-matrix

In describing scattering problems, where one typically considers initial and final configurations of widely separated particles, the description in terms of **in** and **out** states is advantageous. A vector $|a\rangle_{in}$ in Hilbert space corresponds to a physical system characterized by the configuration a at time $t = -\infty$. Similarly a vector $|b\rangle_{out}$ corresponds to a system characterized by the configuration b at time $t = +\infty$. The states $|a\rangle_{in}$ can be counted in the same way as the free particle states:

$$\begin{split} |0\rangle_{in} &= \text{ vacuum at } t = -\infty \\ |\vec{p}_1\rangle_{in} &= \text{ one particle (pion) with momentum } \vec{p}_1 \text{ at } t = -\infty \\ &\dots \\ |\vec{p}_1, \vec{p}_2, \dots, \vec{q}_1, \vec{q}_2, \dots, \rangle_{in} &= \text{ pions with momenta } \vec{p}_1, \vec{p}_2, \dots \text{ and} \\ &\sigma - \text{ particles with momenta } \vec{q}_1, \vec{q}_2, \dots \text{ at } t = -\infty \end{split}$$

A remark needs to be made here.

Since for free particles the energy is known if the three-momentum is known the state is characterized by the three-momenta only. That is why we used the three-vector as argument in $|\vec{p}_1\rangle$ rather than $|p_1\rangle$. In the following we will often drop the arrow, assuming that the reader is aware that the particles indicated are on mass shell($p^2 = m^2$). Note that for finite times, when the particles are not necessarily far apart, the energy is *not simply given* by the usual mass shell relation.

Similarly, for **out** states.

Of course, in general if there is interaction the **in** states are different from the **out** states, although both are in the same Hilbert space. Thus

$$|\vec{p}_1, \vec{p}_2\rangle_{in} \neq |\vec{p}_1, \vec{p}_2\rangle_{out}$$
 (21.73)

because a system that at $t = -\infty$ has two pions with momenta \vec{p}_1 and \vec{p}_2 is unlikely to still have two pions with momenta \vec{p}_1 and \vec{p}_2 at $t = +\infty$. There is some probability that the pions do not scatter; it is given by the absolute value squared of the scalar-product between the two states, that is,

$$\left|_{out} \langle \vec{p}_1, \vec{p}_2 \, | \, \vec{p}_1, \vec{p}_2 \rangle_{in} \right|^2 \tag{21.74}$$

is the probability that, starting with two pions with momenta \vec{p}_1 and \vec{p}_2 at $t = -\infty$ we will still find two pions with momenta \vec{p}_1 and \vec{p}_2 at $t = +\infty$.

Similarly,

$$\left|_{out} \left\langle \vec{p}', \vec{q}\,' \,|\, \vec{p}, \vec{q} \right\rangle_{in} \right|^2 \tag{21.75}$$

is the probability that when measuring on a system characterized by there being two particles of momenta \vec{p} and \vec{q} at $t = -\infty$ we will find two particles of momenta \vec{p}' and \vec{q}' at $t = +\infty$.

We thus have two sets of basis vectors in the same Hilbert space, namely the **in** basis $(|0\rangle_{in}, |\vec{p}_1\rangle_{in},)$ and the **out** basis $(|0\rangle_{out}, |\vec{p}_1\rangle_{out},)$. Since a system without any particles at $t = -\infty$ will still not have any particles at $t = +\infty$, we have $|0\rangle_{in} = |0\rangle_{out}$. Similarly for one particle states, $|\vec{p}_1\rangle_{in} = |\vec{p}_1\rangle_{out}$. But for two or more particle states this is not true if there is any interaction.

Since physical states correspond to vectors of unit length both the **in** and **out** bases are orthonormal. Therefore, there must exist a matrix that transforms the **in** basis into the **out** basis:

$$|a\rangle_{out} = S^+ |a\rangle_{in} \tag{21.76}$$

for any configuration a. We have used S^+ (complex conjugation + transpose = Hermitian) here purely by convention. The *S*-matrix clearly must contain all physical information for any scattering process. For instance, the probability to have configuration a at $t = -\infty$ and to find configuration b at $t = +\infty$ is given by

$$|_{out} \langle b | a \rangle_{in}|^{2} = |_{in} \langle a | b \rangle_{out}|^{2} = |_{in} \langle a | S^{+} | b \rangle_{out}|^{2} = |_{in} \langle b | S | a \rangle_{in}|^{2}$$
(21.77)

The first step is because $\langle a | b \rangle = \langle b | a \rangle^*$, and the last step is nothing but the very definition of S^+ relative to S. Since both **in** and **out** states are orthonormal sets, the S-matrix is unitary (scalar-products are unchanged), so that $S^+S = I$.

Later we will interpret this relation as conservation of probability. If there is no interaction the S-matrix is I (the identity). One therefore often writes

$$S = I + iT \tag{21.78}$$

and the relation $S^+S = I$ becomes

$$i(T - T^{+}) = -T^{+}T \tag{21.79}$$

Exactly the same as in the case of free particle states, we may define matrices a and a^+ in Hilbert space. We can do that on both in and **out** bases. Thus, $a_{in}(\vec{p})$ is a matrix such that

$$a_{in}(\vec{p}) \left| \underbrace{\vec{p}, \vec{p}, \dots, \vec{q}, \dots}_{n \ \vec{p}'s}, \vec{q}, \dots \right|_{in} = \sqrt{n} \left| \underbrace{\vec{p}, \vec{p}, \dots, \vec{q}, \dots}_{n-1 \ \vec{p}'s}, \underbrace{\vec{p}, \vec{p}, \dots, \vec{q}, \dots}_{in} \right|_{in}$$
(21.80)

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Similarly $a_{out}(\vec{p})$ is defined by its action on the unit vectors of the **out** basis.

Note that at this point we have no idea what happens when we apply $a_{in}(\vec{p})$ on some **out** basis vector.

From the $a_{in}(\vec{p})$ and $a_{out}(\vec{p})$ we may construct fields $\varphi_{in}(x)$ (and $\varphi_{out}(x)$) as before:

$$\varphi_{in}(x) = \sum \frac{1}{\sqrt{2Vp_0}} \left(a_{in}(\vec{p})e^{-ipx} + a_{in}^+(\vec{p})e^{ipx} \right)$$
(21.81)

The momentum p refers here to a momentum that can be found with the particles at $t = -\infty$, when they are presumably far apart, and thus their energy will be purely kinetic (no potential energy).

Thus, we then have $p_0 = \sqrt{\vec{p}^2 + M^2}$ for pions and $p_0 = \sqrt{\vec{p}^2 + m^2}$ for σ -particles, which have the field $\sigma_{in}(x)$.

Since the S-matrix transforms the **in** basis into **out** basis it must also transform $a_{in}(\vec{p})$ into $a_{out}(\vec{p})$

$$\begin{split} Sa_{out}(\vec{p})S^{+} \left| \vec{p}, \vec{p}, \dots \right\rangle_{in} &= Sa_{out}(\vec{p}) \left| \vec{p}, \vec{p}, \dots \right\rangle_{out} \\ &= \sqrt{n}S \left| \vec{p}, \dots \right\rangle_{out} = \sqrt{n} \left| \vec{p}, \dots \right\rangle_{in} \\ &= a_{in}(\vec{p}) \left| \vec{p}, \vec{p}, \dots \right\rangle_{in} \end{split}$$

We used $S^{-1} = S^+$ to transform **out** into **in** state. We thus see that

$$a_{in}(\vec{p}) = Sa_{out}(\vec{p})S^+$$
 (21.82)

Similarly

$$\varphi_{in}(x) = S\varphi_{out}(x)S^+ \tag{21.83}$$

Both fields, φ_{in} and φ_{out} satisfy the Klein-Gordon equation.

It must be understood that φ_{in} and φ_{out} are well defined for all space and time. Thus $\varphi_{in}(x)$ for example is perfectly well defined and non-zero for $x_0 = +\infty$.

The essence of the above may be put as follows.

The assumption that for $t = -\infty$ any physical system becomes a system of free particles allows a mapping of all possible physical systems (by how they are at $-\infty$) on all possible free particle systems. Then we can use the formalism developed for those systems, and build fields. The fields so constructed are the **in** fields. Similarly **out** fields, related to labeling physical systems by how they are at $+\infty$. This then exhibits the role of assumptions on asymptotic behavior, which are clearly of fundamental importance.

Let us formulate this once more in different terms.

Consider a physical system as a movie, showing a lot of action as it is projected. This movie is in a can, and the can may be labeled in different ways. The labeling may be on the basis of the opening scene of the movie, or alternatively, on the basis of the final scene.

Clearly, these are very different ways of labeling.

Only empty movies (the vacuum) or movies containing just one actor (one particle of some momentum) are likely to have identical **in** and **out** scenes.

A physical state in Hilbert space is like a movie in a can. It is the whole movie, not just the opening scene, even if the can is labeled that way. Seeing things this way it hopefully becomes clear that a progressing physical system is not a vector in Hilbert space (such as $|\vec{p}, \vec{q}\rangle_{in}$ rotating to another state $(|\vec{p}, \vec{q}\rangle_{out})$ in the course of time.

A vector in Hilbert space has no time dependence, but, like in a movie, all action is contained in that state.

In that sense the S-matrix is a cross-index register, showing the relation between two labeling systems. Given the beginning scene of a movie, the S-matrix tells us what the final scene is.

21.3 Interacting Fields - Part 2

21.3.1 Interpolating Fields

We are now in a position to formulate equations of motion that describe an interaction.

We assume the existence of a field $\varphi(x)$ (no **in** or **out** index) that is equal to $\varphi_{in}(x)$ if x_0 (the time) is $-\infty$ and is equal to $\varphi_{out}(x)$ at $x_0 = +\infty$. Again, $\varphi_{in}(x)$ is well defined at $x_0 = +\infty$, but then it will be very different from $\varphi(x)$. Thus, we have

$$\lim_{x_0 \to -\infty} \varphi(x) = \varphi_{in}(x) \quad , \quad \lim_{x_0 \to +\infty} \varphi(x) = \varphi_{out}(x) \tag{21.84}$$

Figure 21.3 below shows some attempt to visualize the system.

Note that $\varphi_{in}(x)$ and $\varphi_{out}(x)$ are well defined for all times. Now, $\varphi(x)$ will also satisfy an equation of motion, but it will not be a simple Klein-Gordon equation. We therefore write:

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M^2\right)\varphi(x) = -j(x)$$
(21.85)



Figure 21.3: Visualizing "in" to "out"

The minus sign is part of the definition. The quantity j(x) is called a *current*, and j(x) is such that if we solve this equation with the boundary condition

$$\varphi(x) = \varphi_{in}(x) \text{ at } x_0 = -\infty \tag{21.86}$$

then for

$$x_0 = +\infty$$
 we will have $\varphi(x) = \varphi_{out}(x)$ (21.87)

If we know j(x), and can solve this equation then we can find φ_{out} from φ_{in} , and thus also determine the S-matrix since S relates in- and out-fields.

Unfortunately, the equation can be solved only in successive approximations (perturbation theory). We start by assuming that j(x) can be constructed from the φ themselves. This assumption has its basis in the fact that the *a* and a^+ . Since $\varphi(x)$ is to be local (nothing moving with speeds exceeding the speed of light), it makes sense to build up j(x) from the $\varphi(x)$.

Basically all this is one big assumption. The system is really very complicated, even for the simplest cases as we will see. Only for those simple cases can the above equation be solved, and even then only in terms of successive iterations (perturbation theory). Thus the scheme developed below is to a large extent determined simply by the requirement that we can solve it. Fortunately these methods give rise to results that agree very well with experimental observations. One truly may be thankful to nature for this, that is, limiting itself to something that we can compute!

Let us now write down a simple expression for j(x) and solve the equation. Since we want the pions to interact with the σ -particles we will also include σ -fields in j(x). We assume

$$j(x) = -2g\sigma(x)\varphi(x) \tag{21.88}$$

The constant g is called the coupling constant. We will now write $\pi(x)$ instead of $\varphi(x)$ to exhibit more clearly the fact that this particular field is associated with pions.

The above choice is really the simplest non-trivial form for j(x) since if we chose

only $\pi(x)$ or $\sigma(x)$ we could, with some reshuffling of the equation, make j(x) zero and, therefore, this would not correspond to any interactions.

Of course, there is also an equation of motion for the σ -fields:

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - m^2\right)\varphi(x) = -\bar{j}(x)$$
(21.89)

with some other current $\overline{j}(x)$ instead of j(x). As we will see one cannot freely choose $\overline{j}(x)$ if j(x) is already fixed. There is a strong interconnection.

Intuitively, this is simple to see. If j(x) determines how pions interact with σ 's then evidently this fixes also the interaction of σ 's with π 's. In fact, one can determine the S-matrix from either j(x) or $\overline{j}(x)$ above, and this better be the same S-matrix! We will see later that the choice $j = 2g\sigma\pi$ implies $\overline{j} = g\pi^2$.

It should be stressed here that the field $\sigma(x)$ in j(x) is not σ_{in} or σ_{out} but also an *interpolating* field (interpolating between σ_{in} and σ_{out}) just as $\pi(x)$ is an interpolating field (interpolating between π_{in} and π_{out}).

To find the S-matrix we assume the existence of a matrix $U(x_0)$, time-dependent, but not space-dependent, such that:

$$\pi(x) = U^{+}(x_{0})\pi_{in}(x)U(x_{0}) \quad , \quad \sigma(x) = U^{+}(x_{0})\sigma_{in}(x)U(x_{0})$$
(21.90)

Clearly $U(-\infty) = I$ and $U(+\infty) = S$. Since we will explicitly find $U(x_0)$, there is no point in discussing whether this assumption makes sense.

To be complete, it should be noted that from a strict mathematical point of view one can raise many questions and objections, relating to the fact that we are dealing with infinite matrices. But being physicists, we, as usual, ignore these potential problems.

From the fact that $\pi(x)$ satisfies an equation of motion we should be able to deduce an equation of motion for $U(x_0)$. Here we need to be careful because all the objects that we are dealing with are big, generally non-commuting, matrices. Basic equations, derived earlier, that we will use are:

$$\left[\pi(x), \pi(y)\right]_{x_0=y_0} = 0 \quad , \quad \left[\frac{\partial \pi(x)}{\partial x_0}, \pi(y)\right]_{x_0=y_0} = -i\delta^{(3)}(\vec{x} - \vec{y}) \tag{21.91}$$

We will now show that, if $U(x_0)$ satisfies the following differential equation:

$$\frac{\partial U(x_0)}{\partial x_0} = ig \int d^3y \,\pi_{in}^2(y)\sigma_{in}(y)U(x_0) \quad \text{with } y_0 = x_0 \tag{21.92}$$

then $\pi(x)$ as defined above satisfies

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M^2\right)\pi(x) = -2g\sigma(x)\pi(x)$$
(21.93)

The proof of this statement is not particularly difficult, just a little cumbersome. It is important to remember that $U(x_0)$ is time dependent, not space dependent. In other words

$$\frac{\partial U(x_0)}{\partial x_{\mu}} = 0 \ , \ \mu = 1, 2, 3 \tag{21.94}$$

First we introduce a notation:

$$H(x_0) = g \int d^3y \, \pi^2(y) \sigma(y) \quad \text{with } y_0 = x_0 \tag{21.95}$$

and

$$H_{in}(x_0) = g \int d^3y \,\pi_{in}^2(y) \sigma_{in}(y) \quad \text{with } y_0 = x_0 \tag{21.96}$$

It follows that

$$H(x_0) = U^{-1} H_{in}(x_0) U$$
(21.97)

The equation to be solved is now:

$$\frac{\partial U(x_0)}{\partial x_0} = iH_{in}(x_0)U(x_0) \tag{21.98}$$

The time derivative of $\pi(x)$ and $\sigma(x)$ can be computed. Remember, in general:

$$\partial(I) = 0 = \partial(U^{-1}U) = \partial(U^{-1})U + U^{-1}\partial(U) \rightarrow \partial(U^{-1}) = -U^{-1}\partial(U)U^{-1}$$
(21.99)

We then find:

$$\pi = U^{-1} \pi_{in} U \tag{21.100}$$

and

$$\frac{\partial \pi}{\partial x_0} = \frac{\partial (U^{-1}\pi_{in}U)}{\partial x_0} = \frac{\partial (U^{-1})}{\partial x_0} \pi_{in}U + U^{-1}\frac{\partial (\pi_{in})}{\partial x_0}U + U^{-1}\pi_{in}\frac{\partial (U)}{\partial x_0} \\
= -U^{-1}\frac{\partial (U)}{\partial x_0}U^{-1}\pi_{in}U + U^{-1}\frac{\partial (\pi_{in})}{\partial x_0}U + U^{-1}\pi_{in}iH_{in}U \\
= -U^{-1}iH_{in}UU^{-1}\pi_{in}U + U^{-1}\frac{\partial (\pi_{in})}{\partial x_0}U + U^{-1}\pi_{in}iH_{in}U \\
= U^{-1}i[\pi_{in}, H_{in}]U + U^{-1}\frac{\partial (\pi_{in})}{\partial x_0}U \qquad (21.101)$$

We can see a general rule here. The second time derivative of the $\pi-{\rm field}$ becomes:

$$\frac{\partial^2 \pi}{\partial x_0^2} = -U^{-1} \left[\left[\pi_{in}, H_{in} \right], H_{in} \right] U + U^{-1} \frac{\partial}{\partial x_0} i \left[\pi_{in}, H_{in} \right] U + U^{-1} i \left[\frac{\partial \pi_{in}}{\partial x_0}, H_{in} \right] U + U^{-1} \frac{\partial^2 \pi_{in}}{\partial x_0^2} U$$
(21.102)

As noted before the spatial derivatives of U vanish. Considering now the Klein-Gordon equation for $\pi(x)$ we find

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M^2\right)\pi(x) = \left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M^2\right)\left(U^{-1}\pi_{in}U\right)$$
$$= \left(\left(-\frac{\partial^2}{\partial t^2} - M^2\right)U\right)\pi_{in}U$$
$$+ U^{-1}\left(\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M^2\right)\pi_{in}\right)U$$
$$+ U^{-1}\pi_{in}\left(\left(-\frac{\partial^2}{\partial t^2} - M^2\right)U\right)$$
$$= \left(\left(-\frac{\partial^2}{\partial t^2} - M^2\right)U^{-1}\right)\pi_{in}U$$
$$+ U^{-1}\pi_{in}\left(\left(-\frac{\partial^2}{\partial t^2} - M^2\right)U\right)$$
(21.103)

and finally

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M^2 \right) \pi(x) = -U^{-1} \left[\left[\pi_{in}, H_{in} \right], H_{in} \right] U + U^{-1} \frac{\partial}{\partial x_0} i \left[\pi_{in}, H_{in} \right] U + U^{-1} i \left[\frac{\partial \pi_{in}}{\partial x_0}, H_{in} \right] U$$
(21.104)

Since the field π_{in} satisfies the free Klein-Gordon equation, the first term on the right hand side vanishes. Also, the second and third terms vanish because $\pi_{in}(x)$ and $\pi_{in}(y)$ commute for $x_0 = y_0$ (as far as $\pi_{in}(x)$ and $\sigma_{in}(x)$ are concerned, they commute always because the matrices a and a^+ for the π and σ fields commute). The last term gives

$$\begin{bmatrix} \frac{\partial \pi_{in}}{\partial x_0}, H_{in} \end{bmatrix} = ig \int d^3 y \sigma(y) \begin{bmatrix} \frac{\partial \pi_{in}}{\partial x_0}, \pi_{in}^2 \end{bmatrix}_{x_0 = y_0}$$
$$= -2ig \int_{x_0 = y_0} d^3 y \sigma_{in}(y) \delta^{(3)}(\vec{x} - \vec{y}) \pi_{in}(y)$$
$$= -2ig \sigma_{in}(y) \pi_{in}(y) \tag{21.105}$$

The final result is:

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M^2\right)\pi(x) = -2gU^{-1}\sigma_{in}(x)\pi_{in}(x)U$$
$$= -2g\sigma(x)\pi(x)$$
(21.106)

because

$$U^{-1}\sigma_{in}(x)\pi_{in}(x)U = U^{-1}\sigma_{in}(x)UU^{-1}\pi_{in}(x)U = -2g\sigma(x)\pi(x)$$
(21.107)

which is precisely what we set out to prove.

It is then straightforward(same techniques) to show that

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - m^2\right)\sigma(x) = -g\pi^2(x)$$
(21.108)

This is the moment to consider the question of the connection between j and \overline{j} . It is clear from the above derivation that they follow from the same U, i.e., from the same H. As a matter of fact one notes the formal rules:

$$j(x) = \frac{\partial H(x)}{\partial \pi} \text{ and } \bar{j}(x) = \frac{\partial H(x)}{\partial \sigma}$$
 (21.109)

with

$$H(x) = \int d^3 y H(y) , \quad H(y) = g\pi^2(y)\sigma(y)$$
 (21.110)

The quantities H and H are called the interaction Hamiltonian and the interaction Hamiltonian density respectively. It is clear that it is better to start from a Hamiltonian and then to derive the equations of motion to avoid inconsistencies. This is what we will do in general. In fact, at this point we do not really need the equations of motion for the fields any more. We will simply take some Hamiltonian, and we then know that the U-matrix satisfies the equation

$$\frac{\partial}{\partial x_0} U(x_0) = H_{in}(x_0) U(x_0) \tag{21.111}$$

and solve U from that. Once we have U we have the S-matrix, namely, $S = U(\infty)$.

It should be clearly understood what we have here. The solution of the equation for U will give us the matrix U as a function of π_{in} and σ_{in} . Thus we will obtain S as a function of π_{in} and σ_{in} . This is precisely what we need. As noted before, the probability to find the configuration c at time $t = +\infty$ if at time $t = -\infty$ we have the configuration b, is given by

$$\left|_{out} \left\langle c \mid b \right\rangle_{in} \right|^{2} = \left|_{in} \left\langle c \mid S \mid b \right\rangle_{in} \right|^{2} \tag{21.112}$$

We need $_{in} \langle c | S | b \rangle_{in}$ since if S is given in terms of **in** fields we know exactly what S gives when operating on an **in** basis vector.

Thus, in principle there is no problem here. However, the actual calculation of matrix elements $_{in} \langle c | S | b \rangle_{in}$ remains a complicated matter.

The diagram technique introduced by Stuckelberg and Feynman is a very powerful tool to analyze this system. This technique is generally useful for solving equations of the type

$$\frac{\partial X}{\partial t} = AX \tag{21.113}$$

where A is a given, time dependent, quantity. If A s a constant the solution is simple:

$$X = e^{At} \tag{21.114}$$

If A is time-dependent, but not a matrix, just some function, then the solution is:

$$X = \exp\left(\int_{c}^{t} A(t')dt'\right)$$
(21.115)

where c is an arbitrary constant. If A(t) is a matrix such that $A(t_1)$ and $A(t_2)$ do not necessarily commute, then the solution is more complicated and essentially can be given only in terms of a series expansion that looks very much like an expansion of the above exponential, but not exactly (see Chapter 11).

To be precise, it is easy to verify (Chapter 11) that a solution in this case is

$$X = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 \dots \int_{-\infty}^{t} dt_n T(A(t_1)A(t_2)\dots)$$
(21.116)

We have taken the constant c as $-\infty$, to avoid a number of irrelevant complications. The *time ordered* product T is defined as follows. For the product of two A's

$$T(A(t_1)A(t_2)) = \begin{cases} A(t_1)A(t_2) & \text{if } t_1 > t_2 \\ A(t_2)A(t_1) & \text{if } t_2 > t_1 \end{cases}$$
(21.117)

For any number of A's it works similarly, i.e., the A's must be arranged in order of decreasing time. Obviously, if $A(t_1)$ and $A(t_2)$ commute for any t_1 and t_2 then the above expression reduces to an exponential function.

We now proceed to show the correctness of the above solution. It can of course be verified directly by putting the above solution into the equation, but we will use iteration instead. Suppose we want to find X as a power series in A. Let us find the lowest order term. We write $X = 1 + \alpha_1$, where α_1 is of first order in A. Neglecting terms of order A^2 such as $A\alpha_1$ the equation for X becomes

$$\frac{d\alpha_1}{dt} = A \to \alpha_1 = \int_{-\infty}^{t} A(t_1) dt_1$$
(21.118)

To obtain the next iteration we write:

$$X = 1 + \int_{-\infty}^{t} A(t_1)dt_1 + \alpha_2$$
 (21.119)

where α_2 is of second order in A. The equation for X becomes (to second order in A)

$$\frac{d\alpha_2}{dt} = A(t) \int_{-\infty}^t A(t_1) dt_1 \qquad (21.120)$$

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The solution is

$$\alpha_2 = \int_{-\infty}^{t} dt_2 A(t_2) \int_{-\infty}^{t_2} dt_1 A(t_1)$$
(21.121)

Notice that $t_2 > t_1$, that is, the matrices A appear in descending order of time. To further proceed with this integral we claim that

$$\alpha_2 = \int_{-\infty}^t dt_2 \int_{t_2}^t dt_1 A(t_1) A(t_2)$$
(21.122)

also. Note the order of the A and the integration limits of the second integral where again the A appear in descending order. This may be verified either by direct insertion into the equation for $d\alpha/dt$ or by transforming the integral. This becomes very easy by considering Figure 21.4 below showing the integration domains.



Figure 21.4: Integration Domains

Taking c as lower integration limit, with c some number, the first integral corresponds to domain I in the figure and the second to domain II. It is clear that the two domains can be obtained from each other by exchanging t_1 and t_2 . Since indeed the integrands have t_1 and t_2 interchanged we see that the two integrals are equal. We may therefore take also for α_2 half the sum of both expressions and thus obtain

$$\alpha_2 = \frac{1}{2} \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 T(A(t_1)A(t_2))$$
(21.123)

For the sake of clarity we will show directly that the above is the correct solution. First,

$$T(A(t_1)A(t_2)) = \theta(t - t_2)A(t_1)A(t_2) + \theta(t_2 - t_1)A(t_2)A(t_1)$$
(21.124)

This shows *explicitly* the meaning of the T-product. Now,

$$\frac{d\alpha_2}{dt} = \frac{1}{2} \int_{-\infty}^{t} dt_2(\theta(t-t_2)A(t)A(t_2) + \theta(t_2-t)A(t_2)A(t)) + \frac{1}{2} \int_{-\infty}^{t} dt_1(\theta(t_1-t)A(t_1)A(t) + \theta(t-t_1)A(t)A(t_1))$$
(21.125)

Essentially the first part is obtained by setting $t_1 = t$, the second by setting $t_2 = t$. The very first term contains $\theta(t - t_2)$ and is zero unless $t_2 < t$ which is always true since t_2 runs from $-\infty$ to t. We can therefore omit the θ -function in that term, to get

$$\frac{1}{2}A(t)\int_{-\infty}^{t} dt_2 A(t_2)$$
(21.126)

The second term is zero unless $t_2 > t$, which is never true, and that term is zero. Similarly the last two terms, which really differ from the first two only in that the integration variable is called t_1 instead of t_2 . Together we get the desired result.

Similarly, one finds in general:

$$\alpha_n = \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^t dt_2 \dots \int_{-\infty}^t dt_n T(A(t_1)A(t_2)\dots A(t_n))$$
(21.127)

In this case one must consider n! domains of integration, all obtained from each other by some permutation of $t_1t_2....t_n$, but there is no essential difference from the case of just two variables.

21.4 Interacting Fields - Part 3

21.4.1 Feynman Rules

We will now work out the lowest non-vanishing order of the S-matrix for the case of the π and σ fields given before. We have

$$\frac{\partial U(x_0)}{\partial x_0} = iH_{in}(x_0)U(x_0) \tag{21.128}$$

 or

$$\frac{\partial U(x_0)}{\partial x_0} = i \int_{x_0 = y_0} d^3 y \mathbf{H}_{in}(y) U(x_0)$$
(21.129)

In first approximation we find:

$$U(x_0) = 1 + i \int_{-\infty}^{x_0} dt_1 \int_{y_0 = t_1} d^3 y H_{in}(y)$$
(21.130)

where we used y_0 directly instead of t_1 . Note that $d^4y = d^3y dy_0$. The S-matrix follows by taking the limit $x_0 = +\infty$.

$$S = 1 + i \int d^4 y \mathcal{H}_{in}(y) + \dots \dots$$
 (21.131)

The general expression for S is:

$$S = 1 + \sum_{n=1}^{\infty} \frac{i^n}{n!} \int d^4 y_1 d^4 y_2 \dots d^4 y_n T\left(\mathbf{H}_{in}(y_1) \dots \mathbf{H}_{in}(y_n)\right)$$
(21.132)

Let us now concentrate on a specific process. Consider the scattering of two pions with momenta p and q giving rise to two pions with momenta p' and q'. We must calculate:

$$_{out} \langle p', q' \mid p, q \rangle_{in} = _{out} \langle p', q' \mid S \mid p, q \rangle_{in}$$

$$(21.133)$$

with S as above, and

$$H(y) = g\pi_{in}^{2}(y)\sigma_{in}(y)$$
(21.134)

Remember also that

$$\pi_{in}(y) = \sum_{k} \frac{1}{\sqrt{2Vp_0}} (a_{in}(k)e^{-iky} + a_{in}^+(k)e^{iky})$$
(21.135)

where $a_{in}(k)$ transforms a state with m pions into a state with m-1 pions, and gives zero if no pions are present, while $a_{in}^+(k)$ gives the opposite result.

Let us first consider the lowest order term of S. As we have now exclusively in type objects we will drop this subscript. We have:

$$\langle p', q' | S | p, q \rangle = \langle p', q' | p, q \rangle + i \int d^4 y \langle p', q' | H(y) | p, q \rangle$$
(21.136)

plus terms of higher order in H. Now, if p', q' is different from p,q then the first term is zero (orthogonal vectors). The second term contains one H and therefore only one σ field. This applied to a state without σ particles gives zero (for the a(k) part) or a state containing a σ particle. But the dot product of such a state with the state $|p',q'\rangle$, containing no σ particle is zero. Therefore also the second term is zero.

Generally, any product of an odd number of H's gives zero between states without σ particles, by similar arguments.

Let us now consider the second order term. It is given by:

$$\frac{ig^2}{2} \int d^4y d^4y' \langle p', q' | T\left(\pi^2(y)\sigma(y)\pi^2(y')\sigma(y')\right) | p, q \rangle$$
(21.137)

Now we will have non-zero terms. For instance, some a^+ term in the σ -field can transform the state $|p,q\rangle$ into a state containing in addition a σ particle of, say, momentum k, i.e.,

$$\sigma |p,q\rangle = |p,q,k\rangle \tag{21.138}$$

Then two *a*-type terms in the following two π fields may transform this state into a state containing no pions, i.e.,

$$\pi^2 \sigma |p,q\rangle = |k\rangle \tag{21.139}$$

Next the appropriate a(k) term in the σ field transforms this state into the state

$$\sigma \pi^2 \sigma |p,q\rangle = |0\rangle \tag{21.140}$$

Finally, selecting the terms with $a^+(p')$ and $a^+(q')$ in the last two pion fields transforms the state $|0\rangle$ into the state $|p',q'\rangle$. The scalar product of this state with $|p',q'\rangle$ is non-zero; in fact it is one.

This may be graphically depicted in the following way. Particles are described by lines, and the action of σ and π fields is to either end or start a line. The action of H is thus to start or end two π lines and one σ line. The above example, drawn in the opposite direction (i.e. with y' left of y) is shown in Figure 21.5 below.



Figure 21.5: Feynman diagram for $\pi\pi$ scattering

H(y') ends two π lines and starts a σ line corresponding to $\pi^2 \sigma |p,q\rangle = |k\rangle$ and H(y) ends a σ line and starts two π lines.

We now can draw pictures corresponding to all possibilities. They are shown in Figure 21.6 below.

We have drawn the vertices as visible dots, to avoid confusion with crossing lines. The last case shown differs from the first only by the interchange of y and y'. Since the whole is symmetric in y and y' it follows that both cases give the same result. Also the first four diagrams all correspond to the same expression.

All together we get the contributions shown in Figure 21.7 below:



+ further permutations

Figure 21.6: All Possible Feynman diagrams for $\pi\pi$ scattering



Figure 21.7: Different Feynman diagrams for $\pi\pi$ scattering

Generally, in higher orders one gets the same result for all permutations of y, y', y'',, which gives a factor n! for the n^{th} order. This cancels against the factor 1/n! in front.

So far we have not worried about the various factors going with the a and a^+ . This is not very difficult.

Let us take the first diagram shown in Figure 21.8 below.



Figure 21.8: First Feynman diagrams for $\pi\pi$ scattering

We find:

$$\begin{pmatrix} \frac{1}{\sqrt{2Vp_0}} e^{ipy'} \frac{1}{\sqrt{2Vq_0}} e^{iqy'} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2Vk_0}} e^{-iky'} \frac{1}{\sqrt{2Vk_0}} e^{iky} \end{pmatrix} \times \begin{pmatrix} \frac{1}{\sqrt{2Vp'_0}} e^{-ip'y'} \frac{1}{\sqrt{2Vq'_0}} e^{-iq'y'} \end{pmatrix}$$
(21.141)

This is for $y_0 > y'_0$. For $y'_0 > y_0$ the order of the H is reversed, which is of no consequence to the π part, but now the σ starts in the point y and ends in y'.

All together we get:

$$\int d^{4}y d^{4}y' \frac{ig^{2}}{4V^{2}\sqrt{p_{0}q_{0}p_{0}'q_{0}'}} e^{-i(p+q)y'} e^{i(p'+q')y} \times \left(\theta(y_{0}-y_{0}')\sum_{k}\frac{1}{2Vk_{0}}e^{-ik(y-y')} + \theta(y_{0}'-y_{0})\sum_{k}\frac{1}{2Vk_{0}}e^{-ik(y'-y)}\right)$$
(21.142)

Let us now first work out the expression in brackets. The sum over k may be written as an integral over d^3k , and by methods as described before we may rewrite the whole in terms of a 4-dimensional integral.

$$\sum_{k} \frac{1}{2Vk_0} e^{-ik(y-y')} \to \frac{1}{(2\pi)^3} \int d^4k e^{-ik(y-y')} \theta(k_0) \delta(k^2 + m^2)$$
(21.143)

This function is denoted by $\Delta^+(y - y')$. Similarly the second term, differing

only by the interchange of y and y'.

$$\sum_{k} \frac{1}{2Vk_{0}} e^{-ik(y'-y)} \rightarrow \frac{1}{(2\pi)^{3}} \int d^{4}k e^{-ik(y'-y)} \theta(k_{0}) \delta(k^{2}+m^{2}) \qquad (21.144)$$
$$= \frac{1}{(2\pi)^{3}} \int d^{4}k e^{ik(y-y')} \theta(k_{0}) \delta(k^{2}+m^{2})$$
$$= \Delta^{-}(y-y') \qquad (21.145)$$

In the last step we replaced k by -k. One has evidently

$$\Delta^+(z) = \Delta^-(-z) \tag{21.146}$$

The combination

$$\Delta_F(y-y') = \theta(y_0 - y'_0)\Delta^+(y-y') + \theta(y'_0 - y_0)\Delta^-(y-y')$$
(21.147)

is called the *propagator* of the σ -field. It can be worked out easily using a Fourier expression for the θ -function. On has

$$\theta(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\tau \frac{e^{i\tau z}}{\tau - i\varepsilon} \quad , \quad \lim \varepsilon \to 0 \ , \ \varepsilon > 0 \tag{21.148}$$

You can confirm this equation by considering the poles of the integrand in the complex τ plane. Add an integral over a large half circle to make a closed contour; take this circle either in the upper or lower τ plane depending on the sign of z such that the exponential becomes very small on the circle.

With this expression we have:

$$\Delta_F(z) = \frac{1}{(2\pi)^4 i} \int d^4k \int d\tau e^{-ikz + i\tau z_0} \left(\frac{\theta(k_0)\delta(k^2 + m^2)}{\tau - i\varepsilon} + \frac{\theta(-k_0)\delta(k^2 + m^2)}{-\tau - i\varepsilon} \right)$$
(21.149)

The trick is to get τ out of the exponential. This may be achieved by a change of variable for the k_0 integration. We take

$$k_0 = k_0' + \tau \tag{21.150}$$

Note that $kz = k_0 z_0 - \vec{k} \cdot \vec{z}$. We then find

$$\Delta_F(z) = \frac{1}{(2\pi)^4 i} \int d^4k \int d\tau e^{-ikz} \left(\begin{array}{c} \frac{\theta(k_0+\tau)\delta(\vec{k}^2 - (k_0+\tau)^2 + m^2)}{\tau - i\varepsilon} \\ + \frac{\theta(-k_0-\tau)\delta(\vec{k}^2 - (k_0+\tau)^2 + m^2)}{-\tau - i\varepsilon} \end{array} \right) \quad (21.151)$$

where we renamed k'_0 to k_0 . Next we do the τ integral. The argument of the δ -functions is zero if

$$k_0 + \tau = \pm \sqrt{\vec{k}^2 + m^2} = \pm \sqrt{(21.152)}$$

The θ -functions select the + root for the first term and the – root for the second. The argument of the δ -function can be rewritten

$$\vec{k}^2 - (k_0 + \tau)^2 + m^2 = \left(\sqrt{-(k_0 + \tau)}\right)\left(\sqrt{+(k_0 + \tau)}\right)$$
(21.153)

Remember again

$$\delta(ab) = \frac{1}{|a|}\delta(b) + \frac{1}{|b|}\delta(a) \tag{21.154}$$

We find

$$\Delta_F(z) = \frac{1}{(2\pi)^4 i} \int d^4 k e^{-ikz} \frac{1}{2\sqrt{\vec{k}^2 + m^2}} \left(\frac{1}{-k_0 + \sqrt{-i\varepsilon}} + \frac{1}{k_0 + \sqrt{-i\varepsilon}} \right) (21.155)$$

The complete expression for the diagram considered is

$$\frac{ig^2}{(2\pi)^4 i V^2 \sqrt{16p_0 q_0 p'_0 q'_0}} \int d^4k \int d^4y d^4y' \frac{e^{-i(p+q)y'} e^{i(p'+q')y} e^{-ik(y-y')}}{k^2 - m^2 - i\varepsilon}$$
(21.156)

Both y and y' occur only in the exponents, and the integrals can be done using

$$\delta(a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \, e^{-iax} \tag{21.157}$$

and we find

$$\frac{-g^2}{(2\pi)^4 i V^2 \sqrt{16p_0 q_0 p'_0 q'_0}} (2\pi)^8 \int d^4k \frac{1}{k^2 - m^2 - i\varepsilon} \delta^{(4)}(p+q-k) \delta^{(4)}(k-p'-q')$$
(21.158)

The integral over k can be done

$$\frac{-g^2(2\pi)^8}{(2\pi)^4 i V^2 \sqrt{16p_0 q_0 p'_0 q'_0}} \frac{\delta^{(4)}(p+q-p'-q')}{(p+q)^2 - m^2 - i\varepsilon}$$
(21.159)

From the above calculation we can see how things go in general. Write down all possible diagrams, and then for any diagram write down the correct factors. As much as possible factors relating to permutations should be absorbed into some easy rules. This is not always possible, but in most cases that one meets there is really not much of a problem.

First, the combinatorial factor relating to there being two pion lines in a vertex that can be interchanged, is easily taken care of by including a factor of 2 in the vertex. The factor of two relating to the symmetry in y,y' interchange cancels against the factor 1/2! in front of the second order term of the S-matrix expansion. Now we have three essentially different diagrams left:

The contribution due to the first diagram has been computed rules for the theory that we are considering here. Here are the *Feynman rules* for the case $H(x) = g\pi^2(x)\sigma(x)$:

1. To every incoming or outgoing π or σ of momentum p corresponds a factor $1/\sqrt{2Vp_0}$



Figure 21.9: The Essentially Different Feynman diagrams for $\pi\pi$ scattering

- 2. To every vertex corresponds a factor $2i(2\pi)^4g\delta^{(4)}(\dots)$. Note: 2 for two pion lines, i from the original equation for the *S*-matrix, $(2\pi)^4$ from the integral giving the δ -function, and g as found in the interaction Hamiltonian
- 3. To every propagator corresponds a factor

$$\frac{1}{(2\pi)^4 i} \int d^4k \frac{1}{k^2 - m^2 - i\varepsilon}$$
(21.160)

For the pion field one has M^2 instead of m^2

Many of the propagator integrals can usually be done, thereby getting rid of the δ -functions due to the vertices. The general rule is that one $\delta^{(4)}(\dots)$ remains, assuring that the sum of incoming momenta equals the total of the outgoing momenta, thus guaranteeing conservation of energy and momentum in any process. In the first non-trivial order (as we are considering here) no momentum integral remains. In the next order one four-dimensional integral remains non-trivial, and in every next order there is one more four-integral. This is what makes it so hard to do higher order calculations.

21.5 Interacting Fields - Part 4

21.5.1 Feynman Propagator

This is the moment to reflect on the most important central quantity, the Feynman propagator Δ_F . Its definition was

$$\Delta_F(y-y') = \theta(y_0 - y'_0)\Delta^+(y-y') + \theta(y'_0 - y_0)\Delta^-(y-y')$$
(21.161)

The functions Δ^+ and Δ^- are

$$\Delta^{\pm}(y-y') = \frac{1}{(2\pi)^3} \int d^4k \, e^{ik(y-y')} \theta(\pm k_0) \delta(k^2 + m^2) \tag{21.162}$$

In words, one may understand, the Feynman propagator as follows:

If the time y_0 is larger than the time y'_0 then this propagator equals a function containing plane waves for a particle of positive energy on mass shell. We can literally say that if the time $y_0 > y'_0$ then the Feynman propagator represents a physical particle moving from the space-time point y' to the space-time point y. In fact, the exponential is nothing else but the wave function for a plane wave for a particle leaving y' multiplied by the wave function for a particle of the same mass and momentum arriving at y. This product is the overlap of these functions, something that relates to the probability for this to happen. The total propagator is obtained when integrating over all possible physical momenta (positive energy, on mass shell). If the time $y'_0 > y_0$, then the particle moves in the opposite direction.

There is a causality idea in there: energy moves from the earlier point to the later. There is another feature: the probability for this to happen must not be negative, which is embodied in the sign of the Δ^{\pm} . Indeed, having a theory with Δ^{\pm} as above but with a – sign in front would give rise to negative probabilities. This then is the physical content of the Feynman propagator.

The appearance of the θ -functions in Δ_F and Δ^{\pm} thus relates closely to physical concepts. It turns out that these same θ -functions are crucial for the study of unitarity of the *S*-matrix, i.e., conservation of probability. And the sign of the Δ^{\pm} relates to the sign of probability: if it happens to be minus for some particle, then that particle better be a ghost, meaning that the sum total of its effects must somehow cancel. Things like that happen in gauge theories, where then the symmetry of the theory guarantees the necessary cancellations.

21.5.2 Scattering Cross Section

We now introduce a new particle in addition to the π and σ , and we will call it P. Apart from the spin, which one usually neglects in first approximation, this P is to play the role of the proton.

It interacts with the σ in the same way as the π (the electron). Thus the interaction Hamiltonian becomes:

$$H = g\pi^2 \sigma - gP^2 \sigma \tag{21.163}$$

The minus sign reflects the fact that the proton charge is opposite to the electron charge.

We then obtain the following equations of motion:

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M^2\right)\pi(x) = -2g\pi\sigma \qquad (21.164)$$

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - m^2\right)\sigma(x) = -g\pi^2 + gP^2$$
(21.165)

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2 - M_P^2\right) P(x) = 2gP\sigma \qquad (21.166)$$

These follow from previous results, as well as the fact that the P field commutes with all π and σ fields, including time derivatives of these fields. The Feynman rules are as before, except we now have an extra particle, the P, to be denoted by a broken line. There is also a new kind of vertex, showing the $\sigma - P$ coupling as shown in Figure 21.10 below.



Figure 21.10: New Particle Additions

Next we consider πP scattering as shown in Figure 21.11 below.



Figure 21.11: πP Scattering

In this case, to second order, we wind up with only one diagram as shown in Figure 21.12 below.



Figure 21.12: Only 2_{nd} -order diagram in πP Scattering

and the corresponding expression for the S-matrix element, or amplitude, is

$$\langle S \rangle = \frac{(2g)(-2g)i^2(2\pi)^8}{(2\pi)^4 i V^2 \sqrt{16p_0 q_0 p'_0 q'_0}} \frac{\delta^{(4)}(p+q-p'-q')}{(p-p')^2 - m^2 - i\varepsilon}$$
(21.167)

where m is the σ -mass.

To obtain a cross section we must take the absolute value squared of this expression, which is not immediately clear because of the δ -function. To get around this we first go back to finite volume V, which amounts to the replacement

$$\delta^{(3)}(\vec{p} + \vec{q} - \vec{p}' - \vec{q}') \to \frac{V}{(2\pi)^3} \delta_{\vec{p} + \vec{q}, \vec{p}' + \vec{q}'}$$
(21.168)

Thus,

$$(\delta^{(3)}(....))^2 \to \frac{V^2}{(2\pi)^6} \delta_{\vec{p}+\vec{q},\vec{p}'+\vec{q}'}$$
 (21.169)

since there is nothing difficult about squaring a Kronecker- δ , but we now have V^2 instead of V. Recombining one V factor with the δ we have

$$(\delta^{(3)}(\dots))^2 \to \frac{V}{(2\pi)^3} \delta^{(3)}(\dots)$$
 (21.170)

Now what about the fourth δ -function (relating to energy conservation)? Here we must introduce a time interval T. Since with plane waves as we consider here there is really no beginning and end to the scattering process we limit our
observations to a time interval T, and will compute the transition probability per unit of time. Essentially, now things are entirely the same for time and space, and squaring the fourth δ -function gives us a factor $T/2\pi$. The transition probability is therefore

$$\left|\langle S \rangle\right|^{2} = \left|\frac{-4ig^{2}(2\pi)^{4}}{V^{2}\sqrt{16p_{0}q_{0}p_{0}'q_{0}'}}\frac{1}{(p-p')^{2}-m^{2}-i\varepsilon}\right|^{2}\frac{VT}{(2\pi)^{4}}\delta^{(4)}(\dots)$$
(21.171)

We want to compare our results to the classical Rutherford scattering cross section formula, thus we must work this over to a cross section. Imagine the (proton) P to be at rest $(q = (M_P, 0, 0, 0))$ and the (electron) π comes in along the z-axis $(p = (p_0, 0, 0, p_z))$. We thus have a stream of π coming along the z-axis. Since we have one particle in the whole universe the flux (= number of particles per unit surface per unit of time) is v/V where v is the velocity of the π . This velocity is given by

$$v = \frac{|\vec{p}|}{p_0}$$
(21.172)

The cross section is the probability per unit of time, for unit flux, summed over all possible final states. Thus,

$$\sigma_{tot} = \frac{V}{(2\pi)^3} \int d^3p' \frac{V}{(2\pi)^3} \int d^3q' \frac{Vp_0}{|\vec{p}|} \left| \langle S \rangle \right|^2 \frac{1}{T}$$
(21.173)

The integrals with the factors in front are simply the continuum limit of summation over all p' and q'. Thus, we arrive at the equation

$$\sigma_{tot} = \frac{V}{(2\pi)^3} \int d^3 p' \frac{V}{(2\pi)^3} \times \int d^3 q' \frac{V p_0}{|\vec{p}|} \left| \frac{-4ig^2 (2\pi)^4}{V^2 \sqrt{16p_0 q_0 p'_0 q'_0}} \frac{1}{(p-p')^2 - m^2 - i\varepsilon} \right|^2 \frac{VT}{(2\pi)^4} \delta^{(4)} (\dots) \frac{1}{T}$$
(21.174)

or

$$\sigma_{tot} = \frac{16g^2}{(2\pi)^2} \frac{1}{4p_0 q_0} \int d^3 p' \frac{1}{2p'_0} \int d^3 q' \\ \times \frac{1}{2q'_0} \frac{p_0}{|\vec{p}|} \left| \frac{1}{(p-p')^2 - m^2 - i\varepsilon} \right|^2 \delta^{(4)}(p+q-p'-q')$$
(21.175)

The integral over q' can be done, using up three of the δ -functions. We get

$$\sigma_{tot} = \frac{16g^2}{(2\pi)^2} \frac{1}{4p_0 q_0} \int d^3 p' \\ \times \frac{1}{4p'_0 q'_0} \frac{p_0}{|\vec{p}|} \left| \frac{1}{(p-p')^2 - m^2 - i\varepsilon} \right|^2 \delta(p_0 + q_0 - p'_0 - q'_0)$$
(21.176)

where
$$q'_0 = \sqrt{\vec{q}^2 + M^2}$$
 with $\vec{q}' = \vec{p} + \vec{q} - \vec{p}'$.

We now make the non-relativistic approximation and also the no-recoil approximation, which is the approximation that the P mass M_P is much heavier than the mass M of the π .

We then introduce polar coordinates for \vec{p}' , the outgoing π momentum as shown in Figure 21.13 below.



Figure 21.13: π momentum polar coordinates

Then we can write

$$\int d^3p' = \int d\Omega \int y^2 d^3y \tag{21.177}$$

where $y = |\vec{p}|$. Conservation of momentum tells us that q'_0 , the energy of the outgoing P, is given by

$$q_0' = \sqrt{\vec{Q}^2 + M_P^2} \tag{21.178}$$

with Q = p + q - p', and thus

$$\vec{Q} = \vec{p} + \vec{q} - \vec{p}' = \vec{p} - \vec{p}'$$
(21.179)

because $\vec{q} = 0$, as the initial proton is at rest. The quantity \vec{Q} is called the momentum transfer. It is the amount of momentum given by the π to the P.

If M_P is very large we may approximate

$$q_0' = M_P + \frac{\vec{Q}^2}{2M_P} + \dots$$
(21.180)

The no-recoil approximation is to neglect the term

$$\frac{\vec{Q}^2}{2M_P} \tag{21.181}$$

with respect to M_P . Thus, to this approximation the proton remains at rest, $q'_0 = M_P$. The expression for σ_{tot} now becomes

$$\sigma_{tot} = \frac{g^4}{4\pi^2} \frac{1}{p_0 q_0} \int d\Omega \int y^2 d^3 y \frac{1}{4p'_0 q'_0} \frac{p_0}{|\vec{p}|} \left| \frac{1}{Q^2 - m^2 - i\varepsilon} \right|^2 \delta(p_0 - p'_0) \quad (21.182)$$

Now $y = |\vec{p}|$, thus $p'_0 = \sqrt{y^2 + M^2}$. It then follows that

$$\frac{dp'_0}{dy} = \frac{1}{2} \frac{1}{\sqrt{y^2 + M^2}} 2y = \frac{y}{p'_0}$$
(21.183)

or $ydy = p'_0dp'_0$ or $|\vec{p}'|d|\vec{p}'| = p'_0dp'_0$. Furthermore, the δ -function assures us that $p_0 = p'_0$. Thus

$$\sqrt{\vec{p}^2 + M^2} = \sqrt{\vec{p}'^2 + M^2} \tag{21.184}$$

so that $|\vec{p}| = |\vec{p}'|$. We therefore arrive at

$$\sigma_{tot} = \frac{g^4}{4\pi^2} \frac{1}{p_0 q_0} \int d\Omega \int dp'_0 \frac{1}{4p'_0 q'_0} \frac{yp'_0 p_0}{|\vec{p}|} \left| \frac{1}{Q^2 - m^2 - i\varepsilon} \right|^2 \delta(p_0 - p'_0) \quad (21.185)$$

Using the fact that $y = |\vec{p}| = |\vec{p}'|$ and doing the now trivial p'_0 integration we get

$$\sigma_{tot} = \frac{g^4}{4\pi^2} \frac{1}{p_0 q_0} \int d\Omega \frac{p_0}{q'_0} \left| \frac{1}{Q^2 - m^2 - i\varepsilon} \right|^2$$
(21.186)

It should be noted that in the no-recoil approximation $Q_0 \ll |\vec{Q}|$. This follows because Q_0 is the difference between the initial and final P energy

$$Q_0 = q'_0 - q_0 = \sqrt{\vec{Q}^2 + M_P^2} - M_P \approx \frac{\vec{Q}^2}{2M_P}$$
(21.187)

Therefore $Q^2 = \vec{Q}^2$ to a good approximation. Replacing, nonrelativistically, q_0 by M_P and p_0 by M we have the final result

$$\sigma_{tot} = \frac{g^4}{4\pi^2 M_P^2} \int d\Omega \left| \frac{1}{Q^2 - m^2} \right|^2$$
(21.188)

We have omitted the $i\varepsilon$ in the propagator, because both \vec{Q}^2 and m^2 are positive, so the infinitesimal ε is of no relevance here. If we take the σ mass to be zero we have

$$\sigma_{tot} = \frac{g^4}{4\pi^2 M_P^2} \int d\Omega \frac{1}{\vec{Q}^4}$$
(21.189)

Now $\vec{Q} = \vec{p} - \vec{p}'$ and

$$\vec{Q}^2 = 2\left|\vec{p}\right|^2 (1 - \cos\theta) = 4\left|\vec{p}\right|^2 \sin^2\frac{\theta}{2}$$
(21.190)

where we used $|\vec{p}| = |\vec{p}'|$ and θ is the angle that the outgoing makes with the *z*-axis (the direction of the incoming π), Thus

$$\sigma_{tot} = \frac{g^4}{4\pi^2 M_P^2} \int d\Omega \frac{1}{16 |\vec{p}|^4 \sin^4 \frac{\theta}{2}} = \frac{g^4}{64\pi^2 M_P^2 M^4} \int d\Omega \frac{1}{v^4 \sin^4 \frac{\theta}{2}} = \frac{2\pi g^4}{64\pi^2 M_P^2 M^4} \int \frac{\sin \theta d\theta}{v^4 \sin^4 \frac{\theta}{2}}$$
(21.191)

which is indeed the angular distribution as given by the Rutherford scattering formula. In here v is the velocity of the initial π , with $|\vec{p}| = Mv$ as usual and $d\Omega = \sin\theta d\theta d\varphi$.

21.5.3 Lifetime

In this last section we will consider another application of the theory developed so far, namely the calculation of a decay rate, or a lifetime for an unstable particle.

In principle we have here a contradiction. An unstable particle lives a finite time, and therefore it is impossible to be present at either minus or plus infinite time. In other words, an unstable particle will not occur in **in**-states or **out**-states. We will do as if it can be in an **in**-state and then calculate its decay probability. The full justification for that requires a complete treatment of *unstable particles*, which we will not do here.

Going back to the interaction Hamiltonian described before, $H = g\pi^2 \sigma$, we will now consider the case that the σ -particle is heavier than two pions, so that it normally will decay. The decay probability per unit time is called the decay rate, and the inverse of the decay rate is the lifetime.

The process of interest has initially a σ and finally two pions. We therefore must consider

$$\langle p, q | S | k \rangle \tag{21.192}$$

where k denotes the momentum of the initial σ and p and q are the momenta of the final pions.

In lowest order there is one non-vanishing Feynman diagram is shown in Figure 21.14 below.



Figure 21.14: Feynman diagram for σ decay

The corresponding expression is

$$\langle S \rangle = \frac{i (2\pi)^4 2g}{\sqrt{8p_0 q_0 k_0 V^3}} \delta_4 \left(k - p - q\right)$$
(21.193)

The transition probability is

$$|\langle S \rangle|^2 = \frac{(2\pi)^8 4g^2}{8p_0 q_0 k_0 V^3} \frac{V}{(2\pi)^3} \frac{T}{2\pi} \delta_4 \left(k - p - q\right)$$
(21.194)

The transition probability per unit of time follows by dividing by T. We must also sum over all final states if we want the total decay rate. This rate is therefore

$$\Gamma(\sigma \to 2\pi) = \frac{1}{2} \frac{V}{(2\pi)^3} \int d^3 p \frac{V}{(2\pi)^3} \int d^3 q \frac{(2\pi)^8 4g^2}{8p_0 q_0 k_0 V^3} \frac{V}{(2\pi)^3} \frac{1}{2\pi} \delta^{(4)}(k-p-q)$$
$$= \frac{g^2}{(2\pi)^2 k_0} \int d^3 p \frac{1}{2p_0} \int d^3 q \frac{1}{2q_0} \delta^{(4)}(k-p-q)$$
(21.195)

There is a subtlety here, we have divided by 2. This is because the two pions in the final state are identical, and if we integrate over all momenta we will count double, because the final state with the two pions interchanged is the same state (Bose-Einstein statistics). To work out the above expression we go to the a rest system. In this system $k_0 = m$ and $\vec{k} = 0$. This makes the \vec{q} integral trivial, giving $\vec{q} = -\vec{p}$ and therefore $q_0 = p_0$. We get

$$\Gamma(\sigma \to 2\pi) = \frac{g^2}{4\pi^2 m} \int p^2 dp \frac{1}{4p_0^2} \delta(m - 2p_0)$$
(21.196)

We go to polar coordinates. The integral over angles is also trivial giving a factor 4π . We have

$$\Gamma(\sigma \to 2\pi) = \frac{g^2}{4\pi m} \int p^2 dp \frac{1}{p_0^2} \delta(m - 2p_0)$$
(21.197)

Now $p = |\vec{p}|$. Using the relation $pdp = p_0 dp_0$ this last integral is trivial and we obtain

$$\Gamma(\sigma \to 2\pi) = \frac{g^2}{8\pi m} \frac{p}{p_0}$$
(21.198)

with $p_0 = m/2$ and $p = \sqrt{p_0^2 - M^2}$. Thus

$$\Gamma(\sigma \to 2\pi) = \frac{g^2}{8\pi m} \sqrt{m^2 - 4M^2}$$
 (21.199)

The lifetime is the inverse of this, $\tau = 1/\Gamma$.

Numerical Evaluation

Generally one wants a cross section in terms of cm^2 and a lifetime in seconds. We have used h = c = 1 and will express everything else in MeV. The cross section will have the dimension of $(MeV)^{-2}$, the decay rate is of dimension MeV and lifetime $(MeV)^{-1}$. To go to cm^2 the cross section must be multiplied by $(hc)^2 = 1.97327 \times 10^{-11} (MeV - cm)^2$. To go from MeV to sec^{-1} the decay rate must be divided by $h = 6.582122 \times 10^{-22} MeV$ – sec and the lifetime is thus h/Γ . Note that in the examples above the coupling constant g has the dimension MeV.

Chapter 22

The Measurement Problem

The solution to the so-called "quantum measurement" problem is fully developed within the standard structure of quantum mechanics (4 postulates). I have collected together and organized the thoughts of many other physicists (especially Hobson), filled in many details and derivations and generally produced a unified picture of the solution.

22.1 Basic Quantum Mechanics Reviewed

I am assuming that you have already studied the basics of quantum mechanics prior to this discussion.

We can then state the standard formulation of quantum mechanics based on the 4 postulates listed below(with some embellishments):

- All physical systems are represented by ket vectors $|\psi\rangle$ normalized to 1, $\langle \psi | \psi \rangle = 1$. The ket labels represent everything that we know about the system.
- •• Measurable properties of physical systems are represented by linear operators called **observables**.

So restating part of the first postulate, the ket labels represent the values of all observables of the system that have been measured.

If vector associated with particular physical state $|\psi\rangle$ is an eigenvector, with eigenvalue α , of operator \hat{A} associated with particular measurable property of system, i.e., if $\hat{A} |\psi\rangle = \alpha |\psi\rangle$, then the system in that state **has** the value α of that measurable property.

This implies that if one performs a measurement corresponding to the observable represented by \hat{A} on a system in the state $|\psi\rangle$, then with **certainty** (probability =1) the measurement yields the value α for that measurable property.

Observables are represented by Hermitian operators (real eigenvalues). Since the eigenvectors of any Hermitian operator form a complete, orthonormal set, they can be used as a basis for the Hilbert space of the system.

Finally, if the system is in the state $|\psi\rangle$ and one measures an observable \hat{B} , where $|\psi\rangle$ is **not** an eigenvector of \hat{B} , the the only possible results of the measurement are one of the eigenvalues $\{b_k\}$ of \hat{B} .

•• Dynamics of state vectors

The state vectors of any system change with time via **deterministic** laws (similar to classical rules).

We define the **time evolution or development** operator that governs how a state vector changes in time by the relationship

$$A, t + \Delta t \rangle = \hat{U}(\Delta t) | A, t \rangle \tag{22.1}$$

or the state vector at time $t + \Delta t$ is given by the time evolution operator(Unitary) \hat{U} operating on the state vector at time t.

In general, ket labels(which contain whatever we know(have measured) about state) are the only thing that changes.

The time evolution operator is a unitary operator since the state vector must remain normalized to 1, i.e, the vector length cannot change, which is guaranteed by using a Unitary operator. The only changes to state vectors in quantum mechanics are changes in direction.

The time evolution operator is related to the energy operator

$$\hat{U}(t) = e^{i\hat{H}t/\hbar} \tag{22.2}$$

•• Connection with Experiment/Measurements

We have specified above what happens when one measures a certain property of physical system at a moment when state vector of system is an eigenvector of the operator representing that property?

What if one measures a certain property of physical system at a moment when state vector of system does not happen to be an eigenvector of the operator representing that property (which is most of the time)? We need a new assumption. Suppose the system is in the state $|\psi\rangle$, and one carries out a measurement of a property (observable) associated with the operator \hat{B} . We assume the eigenvectors of \hat{B} are the vectors(states) $|b_i\rangle$, which means that $\hat{B}|b_i\rangle = b_i |b_i\rangle$, i = 1, 2, 3... where the b_i are the corresponding eigenvalues.

Quantum theory now assumes that the outcome of measurement is strictly matter of **probability**.

Quantum theory stipulates that the probability that the outcome of measurement of \hat{B} on the state $|\psi\rangle$ (not an eigenvector) will yield the result b_i (remember the only possible results of measurement are the eigenvalues of \hat{B} no matter what state the system is in), is equal to $|\langle b_i | \psi \rangle|^2$ (the Born rule). The probability is given by the absolute square of of the corresponding component!

The quantum mechanics formalism based on these postulates + embellishments correctly predicts experimental results for all known experiments.

Some ideas implied by these rules are:

These rules imply that one cannot say anything definite about the value of the observable represented by \hat{B} when system is in a state $|\psi\rangle$, which is NOT an eigenvector of \hat{B} .

One can only make probability statements.

Before one measures the observable represented by \hat{B} when the system is in a state $|\psi\rangle$, which is NOT an eigenvector of \hat{B} , the system does not have a value of that observable, according to quantum theory!

Our information about any state is only set of probabilities.

But all of your experience says that objects have values for measured quantities before they are measured, i.e., your experience tells you that the observable represented by \hat{B} has a value even if we do not measure it.

That is your view (standard classical view) about what is real and what is not real.

Quantum theory implies you are wrong in both cases!!

22.1.1 Where is the "collapse" postulate?

Since the system has a definite value of the observable represented by B after the measurement, i.e., a pointer points to a value or a counter clicks or a mark is registered on a piece of paper (note that these are all **irreversible** occurences) and there is no mechanism to produce a single value in the rules as presented so far. Most presentations add another rule at this point called **collapse of the state vector**.

It is proposed that the effect of a measurement is to irreversibly change(collapse) the state vector (which was not an eigenvector of \hat{B}) into an eigenvector of \hat{B} (corresponding to the eigenvalue jsut measured) so that it would be observed to have a definite (probability = 1) value for a subsequent measurement of the operator \hat{B} .

This extra rule says that state vector changes(discontinuously) during measurement from representing range of possibilities (superposition of all possible states) to definite state or only one possible outcome.

Which particular eigenvector it gets changed into is determined by outcome of measurement and cannot be known until then!. It cannot be predicted!

I believe that this last rule should not be added.

First of all, no real mechanism is ever given for "how" this process actually takes place, and second no specifications are given as to exactly "when" it occurs.

I will now proceed to develop a proposal for "definite outcomes" without using any "collapse" rule.

22.2 The Measurement Process

We consider a system consisting of a quantum system (Q-system) and a measurement system (M-system).

If the meter, which we assume is initially OFF (state $|0\rangle_M$) was turned ON when system was in $|+\rangle_Q$ state, then according to the above rules the combined system evolves to

 $|+\rangle_Q |0\rangle_M \rightarrow |+\rangle_Q |+1\rangle_M$ i.e., meter (a good working meter) reads +1 (22.3)

Similarly, if the meter turned ON when the system is in the $|-\rangle_Q$ state, then combined system evolves to

 $|-\rangle_Q |0\rangle_M \rightarrow |-\rangle_Q |-1\rangle_M$ i.e., meter (a good working meter) reads -1 (22.4)

This indicates that measurement, within framework of our rules, CORRE-LATES or ENTANGLES the dynamical variables (Q-system) being measured and the macroscopic (M-system) indicator of the meter, which we assume can be directly (macroscopically) observed.

Let us expand the discussion a bit. We have supposed above that the meter has eigenvectors (labelled by the corresponding eigenvalues)

 $|+1\rangle_M \rightarrow$ meter on: reading +1 (22.5)

$$|-1\rangle_M \rightarrow \text{meter on: reading -1}$$
 (22.6)

$$|0\rangle_M \to \text{meter off}$$
 (22.7)

and the system has eigenvectors (labelled by eigenvalues)

$$|+\rangle_O \rightarrow \text{value} = +1$$
 (22.8)

$$|-\rangle_O \rightarrow \text{value} = -1$$
 (22.9)

Now suppose that the initial state of the system is a superposition

$$|\psi\rangle = a |+\rangle_Q + b |-\rangle_Q \tag{22.10}$$

and thus the initial state of the **combined** system is given by

$$|initial\rangle = (a|+\rangle_Q + b|-\rangle_Q)|0\rangle_M \tag{22.11}$$

which represents the system in a superposition state **and** the meter OFF. We are interested in the evolution of this state according to QM. We note as we stated above that, if, instead of above initial state, we started with the initial states

$$|A\rangle = |+\rangle_Q |0\rangle_M \quad \text{OR} \quad |B\rangle = |-\rangle_Q |0\rangle_M$$
(22.12)

and then turn on the meter, these states must evolve as

$$|A\rangle = |+\rangle_Q |0\rangle_M \to |A'\rangle = |+\rangle_Q |+\rangle_M \tag{22.13}$$

$$|B\rangle = |-\rangle_Q |0\rangle_M \to |B'\rangle = |-\rangle_Q |-\rangle_M \tag{22.14}$$

respectively, indicating that the meter measured the appropriate value (the definition of good meter) since system is in eigenstate and has definite value with certainty.

If system is in initial state corresponding to a superposition, however, then the **linearity** of quantum mechanics says it must evolve

$$|initial\rangle = (a|+\rangle_Q + b|-\rangle_Q)|0\rangle_M \to |final\rangle = a|+\rangle_Q|+\rangle_M + b|-\rangle_Q|-\rangle_M \quad (22.15)$$

We note the problem immediately, i.e., the meter has not ended up in a state with a definite value - it remains in a superposition of two macroscopically different pointer readings, which is never observed in the real world.

Hence, if as most physicists assume, the state vector represents a complete description of the Q-system, there seems to be a need for the "collapse" rule to fix the result and obtain "definite" values!

Since we will not be incorporating the "collapse" rule, we must proceed in a different way.

22.2.1 The Density Operator

The problem, as we will now see, lies with assuming that the state vector is the proper way to represent the Q-system during the measurement process.

The expectation value is the average of set of measurement results taken from a collection of systems in same state. A straightforward calculation of the expectation value takes the following form, with \hat{O} being an operator representing the measurement of specific physical variable and $|\phi\rangle$ state vector of each system in collection:

$$\langle \hat{O} \rangle = \langle \phi | \, \hat{O} \, | \phi \rangle \tag{22.16}$$

If we choose **any** set of basis vectors $\{|i\rangle\}$, i = 1, 2, ... for our vector space, we can expand $|\phi\rangle$ and $\langle\phi|$ as

$$|\phi\rangle = \sum_{i} a_{i} |i\rangle \quad , \quad \langle\phi| = \sum_{j} a_{j}^{*} \langle j|$$
 (22.17)

where

$$a_i = \langle i | \phi \rangle \quad , \quad a_j^* = \langle \phi | j \rangle$$
 (22.18)

Plugging these expansions into the expression for the expectation value:

$$\begin{split} \langle \hat{O} \rangle &= \sum_{j} a_{j}^{*} \langle j | \hat{O} \sum_{i} a_{i} | i \rangle = \sum_{j} \left(\sum_{i} a_{j}^{*} a_{i} \langle j | \hat{O} | i \rangle \right) \\ &= \sum_{j} \left(\sum_{i} \langle \phi | j \rangle \langle i | \phi \rangle \langle j | \hat{O} | i \rangle \right) = \sum_{j} \left(\sum_{i} \left[\langle i | \phi \rangle \langle \phi | j \rangle \langle j | \hat{O} | i \rangle \right] \right) \end{split}$$
(22.19)

Now we define a new operator $\hat{\rho} = |\phi\rangle \langle \phi|$, which is just the **projection operator** onto the state $|\phi\rangle$. We can then write the expectation value as

$$\langle \hat{O} \rangle = \sum_{i} \left(\sum_{j} \langle i | \hat{\rho} | j \rangle \langle j | \hat{O} | i \rangle \right)$$
(22.20)

Using the relation

$$\sum_{j}\left|j\right\rangle \left\langle j\right|=\hat{I}$$

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one finds that the expectation value can be written in a very interesting form

$$\langle \hat{O} \rangle = \sum_{i} \langle i | \hat{\rho} \hat{O} | i \rangle = \operatorname{Tr}(\hat{\rho} \hat{O})$$
(22.21)

i.e., the expectation value is given by the sum over the diagonal matrix elements of the operator product $\hat{\rho}\hat{O}$ (the symbol Tr = Trace is just shorthand for the diagonal sum).

The new operator $\hat{\rho}$ is called the **density operator**.

Why bother?

The real power of density operator approach to QM comes when have to deal with situation in which we **cannot be sure what state system is in**(as in the measurement problem).

Imagine we have a whole collection of identical systems, some in $|\phi_1\rangle$, some in $|\phi_2\rangle$, etc. We might not know which system in which state, and might not even know how many systems are in any one state.

Example: Think about a beam of electrons that has not passed through any Stern-Gerlach(S-G) magnets. Chances are that the spin states of the electrons are completely random. Perhaps the best one can know is the probability of finding an electron in any state.

$$P_1 = \operatorname{Prob}(|\phi_1\rangle)$$
, $P_2 = \operatorname{Prob}(|\phi_2\rangle)$, $P_3 = \operatorname{Prob}(|\phi_3\rangle)$, (22.22)

These probabilities have nothing to do with quantum theory; they simply represent our ignorance of the details of what is happening. Thus, they are **not** related to any quantum amplitudes.

Given a situation like this, one should be able to do some useful calculations.

For example, one could work out expectation value of any measurement as follows.

If one can calculate the expectation value of each individual state, then the overall expectation value is simply given by

$$\langle \hat{O} \rangle = P_1 \langle \phi_1 | \hat{O} | \phi_1 \rangle + P_2 \langle \phi_2 | \hat{O} | \phi_2 \rangle + P_3 \langle \phi_3 | \hat{O} | \phi_3 \rangle + \dots + P_n \langle \phi_n | \hat{O} | \phi_n \rangle \quad (22.23)$$

Think back to original definition of expectation value which just represents the average value of measurement. What we have done here is put together the weighted average of the average value for each state, which is just the definition of the overall average value. Now if one constructs a density operator that is given by

$$\hat{\rho} = P_1 |\phi_1\rangle \langle \phi_1| + P_2 |\phi_2\rangle \langle \phi_2| + P_3 |\phi_3\rangle \langle \phi_3| + \dots + P_n |\phi_n\rangle \langle \phi_n|$$
(22.24)

then the expectation value is still given by

$$\langle \hat{O} \rangle = \operatorname{Tr}(\hat{\rho}\hat{O})$$
 (22.25)

as expected.

Some notation: when the density operator takes the form $\hat{\rho} = |\phi\rangle \langle \phi|$ it is said to represent a **pure state** and when the density operator takes the form $P_1 |\phi_1\rangle \langle \phi_1| + P_2 |\phi_2\rangle \langle \phi_2| + P_3 |\phi_3\rangle \langle \phi_3| + \dots + P_n |\phi_n\rangle$ it is said to represent a **mixed state**

22.2.2 A Crucial Example

Consider a box containing a very large number of electrons, each having spin = 1/2. This means that each electron spin can have measurable component $\pm 1/2$ along any direction. Now, suppose the box has a hole so that the electrons can get out and go into a Stern-Gerlach device oriented to measure the z-components of spin(arbitrary choice).

In order to proceed, we need to know how the box of electrons was prepared.

Let us consider two very different cases:

1. In the first case, we fill the box with electrons that have been prepared in a superposition state

$$|\psi\rangle_1 = \frac{1}{\sqrt{2}}(|\uparrow_z\rangle + |\downarrow_z\rangle) \tag{22.26}$$

This preparation can be done by sending the electrons through an xoriented magnet and choosing one of the resulting beams. Thus, in this case, each electron is in the indicated state - each electron is in a superposition of "up" and "down" in the z-direction. We then fill the box with these electrons.

2. In the second case, we send electrons through a z-oriented magnet and collect electron from both beams "z-up" and "z-down". In this case we know that the electrons are either "z-up" OR "z-down", i.e., they each have a definite value - they are not in a superposition. We then fill the box with the two collections of electrons. Remember the electrons in the box in this case are EITHER in the state $|\uparrow_z\rangle$ OR in the state $|\downarrow_z\rangle$.

Now we proceed with the experiment. In case (1) we observe "z-up" 50% of the time and "z-down" 50% of the time and we know that in order to describe this system by a state vector we must say

$$|\psi\rangle_{BOX(1)} = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle + |\downarrow_z\rangle) \to 50\text{-}50 \text{ up-down}$$
 (22.27)

i.e., every electron in the box is in this superposition state.

In case (2)) we observe "z-up" 50% of the time and "z-down" 50% of the time. But we now have a problem. If I did not know that each electron in the box in this case had a definite value, I would be tempted to describe the this system by the same state vector as in case (1). However, we know that is not true! The electrons in case (2) are not each in a superposition but they have definite values!

So, if I measure z-components I cannot tell whether I have case (1) or case (2) and I do not know how to write the state vector for the box in case (2),

But remember how I created the electron in case (1). They all have a definite value of the x-component, namely, "x-up'. So if I subject the electrons coming out of the box in case (1) to a x-measurement instead of a z-measurement, I will end up with only one beam!

However, in case (2), the electron coming out of the box are either "z-up" OR "z-down" each of which is 50-50 in the x-direction and thus I would end up with two beams after the extra measurement!

The different results mean that their states must be described differently in QM.

State vectors do not give us the freedom to do this unless we want to monkey around with relative phases, i.e., we would need to write

$$|\psi\rangle_{BOX(1)} = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle + |\downarrow_z\rangle) \quad , \quad |\psi\rangle_{BOX(2)} = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle + e^{i\alpha} |\downarrow_z\rangle) \tag{22.28}$$

where α is a completely unknown relative phase factor, which must be averaged over during any calculations since it is different for each separate measurement (each member of ensemble). I actually do not think such an object is a legitimate state vector!

If we use density matrices, we have a very different story. For pure state a density operator (or matrix) is defined as

$$\hat{\rho} = |\psi\rangle\langle\psi| \tag{22.29}$$

for some state vector $|\psi\rangle$, i.e., it is the pure state projection operator.

In case (1) this gives

$$\hat{\rho} = \frac{1}{2} (|1/2\rangle \langle 1/2| + |-1/2\rangle \langle 1/2| + |1/2\rangle \langle -1/2| + |-1/2\rangle \langle -1/2|)$$
(22.30)

Derivation of the $\hat{\rho}$ matrix in the (+1/2, -1/2) basis:

$$\rho = \begin{pmatrix} \langle 1/2 | \hat{\rho} | 1/2 \rangle & \langle 1/2 | \hat{\rho} | -1/2 \rangle \\ \langle -1/2 | \hat{\rho} | 1/2 \rangle & \langle -1/2 | \hat{\rho} | -1/2 \rangle \end{pmatrix}$$
(22.31)

Now

$$\langle 1/2 | \hat{\rho} | 1/2 \rangle$$

$$= \langle 1/2 | \frac{1}{2} (|1/2\rangle \langle 1/2 | + |-1/2\rangle \langle 1/2 | + |1/2\rangle \langle -1/2 | + |-1/2\rangle \langle -1/2 |) | 1/2 \rangle$$

$$= \frac{1}{2}$$

$$(22.32)$$

and so on, so that

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 1\\ 1 & 1 \end{pmatrix} \tag{22.33}$$

where the diagonal matrix elements represent probabilities and the off-diagonal matrix elements imply that one will observe quantum interference effects in this system. It is clear that any pure state density operator cannot be written as the sum of pure state projection operators.

In case (2), however, have

$$\hat{\rho} = \frac{1}{2} (|1/2\rangle \langle 1/2| + |-1/2\rangle \langle -1/2|)$$
(22.34)

and

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix} \tag{22.35}$$

which clearly is sum of pure state projection operators. This corresponds to a mixed state. Note that off-diagonals are zero so that this density operator cannot lead to any quantum interference effects.

Remember, this system(case (2)) is such that electrons have values so that the density operator take this form (sum of projection operators)!!

Note that when electrons DO NOT HAVE VALUES (case (1)) the density operator has interference terms and cannot be written as a sum of projection operators - A DIFFERENCE that does not show up when using state vectors!!

We note that if we treat case (2) as pure state with the extra relative phase factor we would obtain:

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & e^{i\alpha} \\ e^{i\alpha} & 1 \end{pmatrix}$$
(22.36)

which becomes

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix} \quad \text{(same result as before)} \tag{22.37}$$

when we average over α .

Now, let us digress to see what happens in a real classical system.

Consider rolling a die which has possible values = 1,2,3,4,5,6 where the probability of occurrence of each value = 1/6. In this case, the die **has** a value before/after each roll so that we have a mixed state where

$$\hat{\rho} = \frac{1}{6} (|1\rangle \langle 1| + |2\rangle \langle 2| + |3\rangle \langle 3| + |4\rangle \langle 4| + |5\rangle \langle 5| + |6\rangle \langle 6|) \quad \text{mixed state} \quad (22.38)$$

and the expectation value of the \widehat{ROLL} operator is given by

$$\langle \widehat{ROLL} \rangle = \frac{1}{6} (1 + 2 + 3 + 4 + 5 + 6) = 3.5 \text{ standard definition}$$
(22.39)

Now any operator can be written as sum of eigenvalues × projections operators(called the spectral decomposition), i.e., for the \hat{B} operator introduced earlier we can write

$$\hat{B} = \sum_{i} b_{i} \left| b_{i} \right\rangle \left\langle b_{i} \right|$$

so that we have for the \widehat{ROLL} operator

$$\widehat{ROLL} = 1 |1\rangle \langle 1| + 2 |2\rangle \langle 2| + 3 |3\rangle \langle 3| + 4 |4\rangle \langle 4| + 5 |5\rangle \langle 5| + 6 |6\rangle \langle 6| \qquad (22.40)$$

The operator product of the density operator and the \widehat{ROLL} operator can be written (using the orthonomality of the basis state vectors) as

$$\hat{\rho} \,\widehat{ROLL} = \frac{1}{6} (1\,|1\rangle\,\langle 1| + 2\,|2\rangle\,\langle 2| + 3\,|3\rangle\,\langle 3| + 4\,|4\rangle\,\langle 4| + 5\,|5\rangle\,\langle 5| + 6\,|6\rangle\,\langle 6|) \quad (22.41)$$

Thus, the expectation or average value is

$$\langle \widehat{ROLL} \rangle = \operatorname{Tr}(\widehat{\rho}\widehat{ROLL}) = \sum_{k} \langle k | \, \widehat{\rho}\widehat{ROLL} \, | k \rangle = \frac{1}{6} (1 + 2 + 3 + 4 + 5 + 6) = 3.5 \quad (22.42)$$

But, in this case, we know the values are real before the measurement, i.e., we are using a macroscopic die with numbers we can see!

Thus, this particular form of a density operator represents that case. The same was true earlier for the electrons in the box when we knew they were either "up" or "down"! **REMEMBER this fact for later.**

If we were to add the "collapse" rule it raises a host of questions: What exactly do we mean, physically and mathematically, by a "collapse during measurement" of quantum system?

Does collapse occur all at one instant?

Wouldn't instantaneous collapse contradict special relativity?

If collapse occurs during a time interval, then what equation describes its timeevolution during that interval? Quantum states are presumed to follow the Schrödinger equation, which prescribes continuous time evolution; how can instantaneous state collapse be reconciled with smooth evolution?

How can we resolve "problem of outcomes" that appears to arise when a superposed quantum's state is measured by "which-state" detector, creating a so-called entangled state of the quantum and the detector that **appears** to be an indefinite superposition of two macroscopically distinct states of a composite system?

Such questions comprise the quantum measurement problem.

We will now continue this discussion of the measurement problem and finally suggest a resolution of problem of definite outcomes that lies entirely within standard quantum physics.

A "quantum measurement" means any quantum process that results in a macroscopic effect, regardless of whether humans or laboratories are involved.

Thus not only is an electron striking a laboratory viewing screen and creating a visible flash a measurement, but also a cosmic-ray muon striking and macroscopically moving a sand grain on a planet in some other galaxy is a measurement.

To analyze a measurement, we look at a specific experiment: suppose an electron beam passes through a pair of double slits and then impacts a viewing screen. Just as in Thomas Young's similar double-slit experiment using light, performed in 1801, a pattern is formed on the viewing screen that shows interference between two portions of electron beam which are seemingly coming through the two slits: a broad dark-and-bright striped pattern spreads out widely on the screen - much wider than slits - indicating regions of destructive (dark) and constructive (bright) interference.

On closer inspection, the bright lines are formed by a very large number of tiny individual electron impacts, each one making a small flash on the screen.

According to above definition, each flash is measurement of the position of an electron as hits the screen.

Each electron's flash on screen is a measurement!

For the purposes of this analysis, however, it is better to consider a related example of measurement, still based on the double-slit experiment.

Suppose an electron detector is installed at the slits and assume that the detector can detect the electron's position as it passes through slits while disturbing each electron only minimally (in the precise sense described below). Measurement, even by such a minimally-disturbing "which-path detector", changes everything.

Exactly when the detector turns on, the pattern on screen changes from a striped interference pattern to a smoothly-spread-out sum of two single-slit patterns, each showing diffraction but no interference.

The interference pattern abruptly vanishes.

An analogous experiment has been done using light (photons) instead of electrons, and using an interferometer rather than double-slit interference setup.

A which-path detector was randomly switched on or off as each photon passed through this experiment; photons for which the detector was "off" formed an interference pattern while photons for which the detector was "on" formed the expected no-interference pattern.

Reminder:

If the system is in a "pure" superposition state, then the density operator take form

$$\hat{\rho} = \frac{1}{2} (|1/2\rangle \langle 1/2| + |-1/2\rangle \langle 1/2| + |1/2\rangle \langle -1/2| + |-1/2\rangle \langle -1/2|)$$
(22.43)

i.e., sum of projection operators and "cross-terms" (interference terms) or the matrix form

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 1\\ 1 & 1 \end{pmatrix} \tag{22.44}$$

where the diagonal matrix elements represent probabilities and the off-diagonal matrix elements imply that one will observe quantum interference effects in this system. Clearly, any pure state density operator cannot be written as the sum of pure state projection operators.

If in a "mixed state", then the density operator takes the form

$$\hat{\rho} = \frac{1}{2} (|1/2\rangle \langle 1/2| + |-1/2\rangle \langle -1/2|)$$
(22.45)

or the matrix form

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix} \tag{22.46}$$

i.e., sum of projection operators (no interference terms).

As we found in the dice example:

$$\hat{\rho} = \frac{1}{6} (|1\rangle \langle 1| + |2\rangle \langle 2| + |3\rangle \langle 3| + |4\rangle \langle 4| + |5\rangle \langle 5| + |6\rangle \langle 6|) \quad \text{mixed state} \quad (22.47)$$

When we see a quantum system evolve into a "mixed state" density operator, then the quantum system can be interpreted "classically", i.e., a measurement has taken place and it has be irreversibly recorded.

This is the important point!!

22.3 Look closely at "which-path" experiments

In the so-called "delayed-choice" two-slit experiment mentioned above, collapses were instantaneous to within the accuracy of fast switching between the two states; in addition, each collapse is executed entirely while the photon was inside the interferometer.

We can gain considerable insight by studying how quantum theory describes a which-path measurement. Note: it is a measurement as defined earlier, because the detector registers "slit 1" or "slit 2" macroscopically for each electron.

We denote the state of one electron passing through slit 1 as $|\psi_1\rangle$ and the state of one electron passing through slit 2 as $|\psi_2\rangle$. John von Neumann, who was the first to carefully analyze measurement in purely quantum-theoretical terms, insisted on treating not only the measured quantum but also the macroscopic detector as quantum systems because, after all, detectors are made of atoms and they perform a quantum function by detecting individual quanta.

Now let us repeat the earlier discussion again, filling in any remaining gaps and confusions.

Accordingly, one represents the "ready to detect" quantum state of detector by $|ready\rangle$, and the state of detector after detecting an electron by $|1\rangle$ if $|\psi_1\rangle$ was detected, and by $|2\rangle$ if $|\psi_2\rangle$ was detected. A properly operating detector will surely transition from $|ready\rangle$ to $|1\rangle$ upon measurement of an electron that has been prepared (perhaps by simply shutting slit 2) in state $|\psi_1\rangle$.

As a limiting idealization, we assume, with von Neumann, that the measurement of an electron prepared in state $|\psi_1\rangle$ leaves electron still in state $|\psi_1\rangle$ after detection. Such a minimally-disturbing measurement would cause the electron-plus-detector composite system, initially in composite state $|\psi_1\rangle$ (ready), to transition into the final state $|\psi_1\rangle|1\rangle$.

We summarize the process as

$$|\psi_1\rangle |ready\rangle \to |\psi_1\rangle |1\rangle \tag{22.48}$$

Similarly, a minimally-disturbing measurement of and electron initially prepared in $|\psi_2\rangle$ is described mathematically by

$$|\psi_2\rangle |ready\rangle \rightarrow |\psi_2\rangle |2\rangle$$
 (22.49)

Now suppose that both slits are open so each electron can pass through either slit, and suppose the preparation and experiment (e.g. slit widths) is symmetric with respect to two slits. Then the state of each electron as it approaches the slits prior to detection must be described by symmetric superposition

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle) \tag{22.50}$$

But quantum physics, including its time dependence, is **linear**. This imply that $|\psi\rangle |ready\rangle$ evolves according to

$$\begin{aligned} |\psi\rangle |ready\rangle &= \frac{1}{\sqrt{2}} (|\psi_1\rangle + |\psi_2\rangle) |ready\rangle \\ &= \frac{1}{\sqrt{2}} (|\psi_1\rangle |ready\rangle + |\psi_2\rangle |ready\rangle) \\ &\to \frac{1}{\sqrt{2}} (|\psi_1\rangle |1\rangle + |\psi_2\rangle |2\rangle) \end{aligned} (22.51)$$

The final state

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|\psi_1\rangle |1\rangle + |\psi_2\rangle |2\rangle)$$
(22.52)

following detection said to be "entangled" because it cannot be factored into simple product of states of two sub-systems. As indicated in Figure 22.1



Figure 22.1:

when two independent quanta pass near each other, interact, and subsequently separate, the interaction generally entangles the two quanta and entanglement then persists after interaction regardless of how far apart two quanta might eventually travel, provided only that two quanta experience no further interactions.

Despite possibly wide spatial separation, entangled quanta have a unity not possessed by non-entangled quanta.

This unity is source of quantum non-locality.

Entanglement is ubiquitous in nature.

The entangled "measurement state" (22.52) that is at the heart of quantum measurement is remarkably subtle.

To fully understand "entanglement", we first need to understand "superposition".

The quantum principles says that **any** linear combination of possible quantum states of a system, as in (22.50) and (22.52) for example, is also a possible quantum state of that system. Figure 22.2 pictures an experiment that demonstrates such a superposition of states.

This represents a layout of optical paths called a "Mach-Zehnder interferometer.".



Figure 22.2:

A light beam enters at the lower left passing through the "beam splitter" BS1; the reflected beam makes a right angle with the incoming direction, while the transmitted beam passes straight through. So the beam splits and each "half" traverses one of two paths; mirrors M bring the paths back to crossing point as shown.

Devices called "phase shifters", denoted by φ_1 and φ_2 , are placed into each path. The phase shifter can add a short variable length to a path. The second beam splitter BS2 can be placed at crossing point. Without BS2, each "half"-beam moves straight ahead along one path to detector on that path.

Things get more interesting with BS2 in place.

Because 50% of each of two beams then goes to each detector, BS2 mixes two beams together so one can show interference.

The interferometer is constructed so that, when the phase shifters are set to zero, the two "optical paths" (number of wavelengths, after accounting for phase changes upon reflection and refraction) from entry point to D1 are equal while two optical paths to D2 differ by half a wavelength.

It is thus found that the light interferes constructively at D1 and destructively at D2, i.e., all light goes to D1. If one then uses φ_1 or φ_2 to add a half wavelength to either path, the light then interferes constructively at D2 and destructively at D1, i.e., all light goes to D2.

As one continuously varies the length of one or other path by varying one or other phase shifter, one finds that the amount of light arriving at D1 varies continuously from 100% down to 0%, while amount arriving at D2 varies from 0% to 100%.

The two paths are clearly interfering!

The experiment is an interferometer-based analog of Young's double-slit interference experiment demonstrating the wave nature of light.

But, as we know, light is really just photons, and photons are indivisible.

How does nature explain this experiment when we dim the light to point where only one photon at a time traverses the interferometer?

After all, the photon still traverses BS1, yet it cannot split in two because a quantum is unified and cannot be split!

With BS2 removed, one finds either D1 or D2 registers a single entire photon, randomly, with 50-50 probabilities, regardless of how the phase shifters are set.

The randomness is absolute. It is more random than any human macroscopic game, such as coin flips, that only mimics randomness. Nature invents quantum randomness to deal with obstacles such as beam splitters while preserving unity of quantum.

The detectors never register half of a photon. They get either a whole photon or no photon.

What happens in the single-photon experiment with BS2 present?

As discussed earlier, beginning from equal path lengths, which gives constructive interference at D1 and destructive interference at D2, as phase shifters vary, probabilities of detecting photon at D1 and D2 vary as Figure 22.3 which gives the percentage of photons impacting D1.

Importantly, the results do not depend on which phase shifter the experimenter chooses to vary. Since each photon responds to changes in either path length, each photon must follow both paths! This verifies the superposition principle and shows that quanta can be in two places at same time!

This seems paradoxical if we assume photons are tiny particles, but if we assume the photons are waves it is not paradoxical, i.e., each photon simply spreads along both paths, interfering with itself at D1 and D2. One must conclude that each photon travels both paths even when BS2 is not present because once photon enters interferometer must behave in same manner regardless of whether BS2 is placed or not placed at far end.

A delayed-choice experiment provides further evidence for conclusion:

Since photons "do not know" whether BS2 will be inserted, they must travel both paths on all trials including those for which BS2 not inserted - this is connected with entanglement.



Figure 22.3:

With BS2 removed, the situation is like the double-slit experiment with a whichslit detector present:

Each photon is entangled with the macroscopic detectors D1 or D2 as in (22.52). With BS2 present, the two paths mix and we have a situation like double-slit experiment with no which-slit detector:

Each photon follows two paths to each detector where it interferes with itself, and one detects the interference state (22.50).

All of this suggests that measurements affect superposed quantum states via entanglement of the superposed quantum with a detector.

22.4 Resolving Paradoxes and Understanding Measurement

22.4.1 The apparent paradox of Schrödinger's cat

A cat is penned up in a steel chamber, along with the following device:

In a Geiger counter there is tiny bit of radioactive substance, so small, that perhaps in course of an hour one of its atoms decays, but also, with equal probability, perhaps none decay; if it happens, the counter tube discharges and through a relay releases a hammer which shatters a small flask of hydrocyanic acid(poisonous).

If one left the entire system to itself for hour, we would say that cat still lives if no atom has decayed!

If one uses a state vector approach to understanding the entire system, one would express this by having a living and a dead cat mixed or smeared out in equal parts - a superposition of "dead" and "alive"! It is typical of these cases, that the indeterminacy originally restricted to the atomic domain becomes transformed into macroscopic indeterminacy, which can only then be resolved by direct observation, which prevents us from naively accepting as valid the "blurred model" for representing reality.

Mathematically, the nucleus and the cat have become entangled in measurement state (22.52), with $|\psi_1\rangle$ and $|\psi_2\rangle$ representing undecayed and decayed states of nucleus and $|1\rangle$ and $|2\rangle$ representing alive and dead cat.

According to Schrödinger's understanding of situation, the indeterminacy of the nuclear state "becomes transformed into macroscopic indeterminacy" of cat, and since he could not comfortably accept this as "blurred" state", i.e., a cat that is in a superposition of being both alive and dead, he hoped this would say something is wrong with QM.

As we will show, according to standard quantum physics, Schrödinger's 1937 understanding was incorrect:

The composite system (cat-plus-nucleus) is not predicted to be in superposition of two states of a cat, or a nucleus, or a composite system.

Instead, the composite system is predicted to be in a superposition of two **correlations** between cat and nucleus, one in which a live cat is 100% correlated with an undecayed nucleus, and second in which a dead cat is 100% correlated with a decayed nucleus.

Entanglement has transformed a pure state superposition of nuclear states to pure state superposition of correlations between subsystem states.

We will see that this is precisely what one expects, and it is not paradoxical!!

This so-called "problem of definite outcome" applies of course to more than Schrödinger's dramatized example.

Regardless of whether the measuring instrument is a which-slit detector, a

Geiger counter, or a cat, the entangled state (22.52) applies. This state appears at first glance to represent a quantum superposition in which the detector is in two macroscopically different states simultaneously. If so, then there is an inconsistency within quantum physics, because obviously it cannot be this easy to create a macroscopic superposition.

Is it true that (22.52) really represents a macroscopic superposition?

There is more to this entangled state than meets the eye.

If one assumes the detector to be in superposed state $a|1\rangle + b|2\rangle$, one finds that (22.52) necessitates either a = 0 or b = 0, implying that detector is not in an individually superposed state within its own Hilbert space.

The same applies to detected quantum:

It is not in a superposed state $a |\psi_1\rangle + b |\psi_2\rangle$ with both $a \neq 0$ and $b \neq 0$.

The entanglement process leaves neither sub-system superposed!

So far as I know, this simple fact has long been ignored by analysts of measurement problem.

22.4.2 Density Operator to the Rescue

The density operator formalism(discussed earlier) for quantum physics provides a stronger version of this conclusion.

The density operator for a quantum system whose state is $|\psi\rangle$ is simply the projection operator

$$\hat{\rho} = |\psi\rangle \langle \psi| \tag{22.53}$$

As we saw earlier, if the system is in state whose density operator is $\hat{\rho}$, then standard quantum expectation value $\langle \hat{O} \rangle$ of arbitrary observable \hat{O} is found from

$$\langle \hat{O} \rangle = \operatorname{Tr}(\hat{\rho}\hat{O})$$
 (22.54)

This approach is especially useful if the quantum system is a composite of two subsystems A and B.

We define the density operator $\hat{\rho}_A$ for subsystem A alone by by

$$\hat{\rho}_A = \operatorname{Tr}_B(\hat{\rho}) \tag{22.55}$$

where Tr_B means that trace taken only over states of subsystem B.

It is then easy to show(see later) that standard quantum expectation values for

subsystem A alone (values obtained by an observer of A without any knowledge of B) are

$$\langle \hat{O}_A \rangle = \text{Tr}(\hat{\rho}_A \hat{O}_A) \tag{22.56}$$

where \hat{O}_A means any observable operating on system A alone (i.e., operating within A's Hilbert space). Applying this formulation to measurement state (22.52), the reduced density operators for the quantum system (call it A) and its detector (call it B), respectively, are

$$\hat{\rho}_A = \frac{1}{2} (|\psi_1\rangle \langle \psi_1| + |\psi_2\rangle \langle \psi_2|)$$
(22.57)

$$\hat{\rho}_B = \frac{1}{2} (|1\rangle \langle 1| + |2\rangle \langle 2|) \qquad (22.58)$$

The plus signs in (22.57) and (22.58) make one think of superpositions such as (22.50), but these are not superpositions. The density operator for the superposition (22.50) has cross-terms:

$$\hat{\rho} = (|\psi\rangle \langle \psi|) = \frac{1}{2} (|\psi_1\rangle \langle \psi_1| + |\psi_1\rangle \langle \psi_2| + |\psi_2\rangle \langle \psi_1| + |\psi_2\rangle \langle \psi_2|)$$
(22.59)

The two cross-terms, involving both $|\psi_1\rangle$ and $|\psi_2\rangle$, are missing from (22.57). So (22.57) does not describe system in superposition of two quantum states.

However, (22.57) is precisely the density operator one should use if one **knows** the quantum system is either in state $|\psi_1\rangle$ or in state $|\psi_2\rangle$ but one didn't know which and so, due your own to lack of information, you simply assign probability of 1/2 to each of two possibilities.

The same goes for (22.58).

(22.57) and (22.58) are "classical" probabilistic states - analogous to the "states of knowledge" one would assign to coin flip when you know the outcome to be either heads or tails with equal probability but don't know which has occurred.

The situation described by a density operator such as (22.57) is known as "mixture" of states $|\psi_1\rangle$ and $|\psi_2\rangle$, as distinct from "superposition" of states as observed in the Mach-Zehnder experiment and represented by (22.50).

Equation (22.56) tells us that all correct statistics for subsystem A alone can be found from standard formula (22.54) applied to subsystem A alone.

But we have just seen that (22.57) is the density operator one should use if one knows A to be in either $|\psi_1\rangle$ or $|\psi_2\rangle$ without knowing which.

The same goes for subsystem B and (22.58).

In the case of Schrödinger's cat, it follows that the observer of the cat alone sees

outcomes appropriate to a cat that is either alive or dead, **not** both.

For subsystems, the interference terms are missing, and an "ensemble" of repeated trials must exhibit a nonsuperposed mixture rather than superposition.

This is the clear prediction of quantum physics for the entangled state (22.52).

But one must be careful, because (22.57) and (22.58) are not complete descriptions of quantum states of nucleus or cat.

In fact, (22.57) and (22.58) are not quantum states at all but merely "reduced states" arising from actual state (22.52) of composite system when one part of the composite system is removed from the equations.

In case of Schrödinger's cat, (22.57) and (22.58) give the correct predictions for observations of either nucleus alone or cat alone, but do not represent the state of either subsystem because this is given by (22.52).

In fact, when two quanta entangled, neither one has a quantum state of its own!

Physicists, philosophers and mathematicians who specialize in quantum foundations have in past objected to argument that reduced density operators can be adduced in this manner to clarify measurement problem.

They offer two key objections:

First, "basis ambiguity", charges that 'the 'basis set" (set of orthogonal eigenvectors) for operator (22.58) (for example) is entirely ambiguous, so (22.58) cannot represent true quantum state.

It is true that (22.58) doesn't represent true state of the subsystem, because (22.58) is actually just identity operator $|1\rangle\langle 1| + |2\rangle\langle 2|$ in B's subspace, divided by 2, so that any other orthogonal basis set could be used instead. Given only the description (22.58), subsystem B could just as well be described by any other pair of orthonormal vectors in B's subspace, for example

$$\frac{1}{\sqrt{2}}(|1\rangle \pm |2\rangle) \tag{22.60}$$

But B's state of affairs is certainly not entirely described by (22.58). Rather, it is described by composite state (22.52). Equation (22.58) merely tells us following:

If the cat and the nucleus are in state (22.52) then, when one looks at the cat, one is going to see cat that is either alive or dead. There is no claim that (22.58) represents complete quantum state of the cat.

That is, there is no claim that cat is really in either state $|1\rangle$ or state $|2\rangle$, because the state it's really in is admittedly (22.52).

Thus, the basis ambiguity objection to our conclusion (namely, that Schrödinger's cat is either alive or dead, not both) fails.

The second key objection is that (22.57) and (22.58) are "improper density operators" because they arise not from insufficient knowledge (as classical probabilities arise) but from reductions of the full density operator for state (22.52) to Hilbert subspaces of each subsystem. It's true that these reduced density operators do not arise from insufficient knowledge about an actual state.

In fact, we do have complete knowledge of the state of both A and B, namely, the measurement state (22.52). So this objection fails not because it is false but because it is irrelevant:

Reduced operators admittedly do not represent the state of the composite system. They tell us only what we will observe at the nucleus and at the cat and they tell us nothing about the correlations between these observations, so these density operators do not tell us the real state of system.

And so plot thickens.

The entangled state (22.52) properly describes both individual subsystems.

However, the plus sign in (22.52) signifies superposition of two terms. We know, however, that neither subsystem A nor subsystem B is superposed.

What then is meaning of plus sign?

This superposition arose from the superposition represented by (22.50).

We cannot logically ignore this fact - a strategy known as the "shut up and calculate" approach to quantum measurement.

Instead, we must ask: Exactly what is superposed when the two subsystems are in this entangled state?

Superpositions preserve the all-important unity of quantum.

When Max Planck proposed in 1900 that electromagnetic radiation occurs in energy steps of magnitude $E = h\nu$, he tacitly implied the central quantum principle:

The unity of an individual quantum.

Energy (electromagnetic energy in case of radiation) comes in spatially extended

bundles, each having a definite and identical quantity of energy. One cannot have half a quantum, or 2.7 quanta!

You must have either 0 or 1 or 2 etc., quanta. In its own way, this is a fairly natural notion - apparently nature prefers to sub-divide the universe into a countable or even a finite set of entities as opposed to an uncountable continuum!

The spatial extension of these bundles then implies nonlocality:

If we have one quantum and destroy it (by transforming it to something else), we must destroy all of it everywhere simultaneously, because we cannot, at any time, have just part of quantum in existence.

Louis de Broglie put it perfectly in 1924, regarding another kind of quantum namely the electron:

The energy of an electron is spread over all space with a strong concentration in a very small region....That which makes an electron an atom of energy is not the small volume that it occupies in space - I repeat it occupies all space - but the fact that it is indivisible, that it constitutes a unit.

When one transforms the state of a quantum, one must transform the entire extended quantum all at once. Hence there are quantum jumps. Furthermore, composite entangled systems such as atoms also behave in unified fashion.

This unity is the source of the nonlocality seen in experiments involving entangled pairs of photons.

Nonlocality is exactly what one would expect, given the unity and spatial extension of quantum and unitary (i.e. unity-preserving) nature of entanglement process.

Standard nonrelativistic quantum theory prescribes two kinds of time evolution: collapse upon measurement, and Schrödinger equation between measurements.

The key feature of Schrödinger equation is that it prescribes a so-called "unitary" time evolution, meaning time evolution that preserves pure states, i.e., transforms unit Hilbert space vectors into other unit vectors.

Ideas required physically by unity of quantum: If quantum described by pure quantum state at t = 0, should remain pure at later times. This notion prompts us to ask whether measurement process also preserves pure states.

At least in case of the idealized process described in (22.51), the answer is "yes" because both "before" and "after" states are pure.

Measurement state (22.52), since it is pure, represents a highly unified state of affairs, even though one of its subsystems is a macroscopic detector. Thus one suspects that this state, like its progenitor (22.50), is truly a superposition in which the superposed terms represent two situations or states of the same object.

But precisely what is that object, i.e., what is superposed?

We have seen that the states of subsystem A are not superposed, nor are states of subsystem B.

The conventional interpretation (which, as we will see, is subtly incorrect) of a product state such as $|\psi_1\rangle|1\rangle$ is that it represents a state of a composite system AB in which subsystem A is in state $|\psi_1\rangle$ while B is in state $|1\rangle$.

In this case, (22.52) would represent a superposition in which AB is simultaneously in state $|\psi_1\rangle|1\rangle$ and also in state $|\psi_2\rangle|2\rangle$.

The situation of Schrödinger's cat would be: live cat and undecayed nucleus superposed with dead cat and decayed nucleus.

This is at least as physically outrageous as a live cat superposed with a dead cat, and it contradicts the physical implications (a cat that is either alive or dead) of reduced states (22.57) and (22.58) as described earlier.

Something is still wrong!

22.5 Repetition and Intricate Details

Proposal:

The solution to the so-called quantum measurement problem is completely contained within standard quantum mechanics and needs no elaborate new structures and interpretations.

22.5.1 Remember the standard discussion from earlier:

Total system T = quantum system S (states $|s_i\rangle$) + measuring device A (states $|a_i\rangle$), where $|a_0\rangle$ = state of measuring device "OFF". The unitary time evolution rule says that $|s_1\rangle|a_0\rangle \rightarrow |s_1\rangle|a_1\rangle$ and $|s_2\rangle|a_0\rangle \rightarrow |s_2\rangle|a_2\rangle$. The linearity of QM the says that

$$|\psi\rangle_{SA} = (c_1|s_1\rangle + c_2|s_2\rangle)|a_0\rangle = c_1|s_1\rangle|a_0\rangle + c_2|s_2\rangle|a_0\rangle \rightarrow c_1|s_1\rangle|a_1\rangle + c_2|s_2\rangle|a_2\rangle$$

In this derivation

 $|\psi\rangle_S = (c_1 |s_1\rangle + c_2 |s_2\rangle$

is state of the quantum system(superposition), while

$$|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$$

is state of the combined system(superposition).

The quantum measurement problem is the observation that the state

$$|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$$

is not observed as the outcome of the measurement!

What is seen is not a so-called superposition, but either

$$|s_1\rangle |a_1\rangle$$
 or $|s_2\rangle |a_2\rangle$

That is "problem of outcomes".

State

$$|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$$

is usually referred to as a superposition, which is misleading.

Entanglement outweighs superposition as the defining feature of this state. Without entanglement-correlations, we would not have a measurement problem!

Careful investigation of this state in a 2007 experiment(Roch) (Wheeler delayed choice experiment) demonstrates its strikingly non-local character:

A photon jumps from state $|\psi\rangle_S = (c_1 |s_1\rangle + c_2 |s_2\rangle$ to state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ precisely when A(the measuring device) switches on and while photon is still inside the interferometer, and jumps from $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ to $|\psi\rangle_S = (c_1 |s_1\rangle + c_2 |s_2\rangle when A switches off.$

Quantum jumps, removal of interferences, and the observed non-locality are due to entanglement.

Of course, an entangled state = superposition, but it is a very special superposition.

To call $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ simply a "superposition" misses the crucial physics of entanglement and makes all the difference in the understanding of the state.

Entanglement is a characteristic trait of quantum mechanics; one that enforces the entire departure from classical lines of thought.

It is well known that, for 2-part systems, all non-product states exhibit nonlocality (Bell inequality).

Thus when S and A are entangled $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$, they share a non-local channel.

The measurement state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ is subtle. Although $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ is called a superposition of S and/or superposition of A, neither is true.

When S and A in measurement state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ neither S nor A in superposition. $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle =$ superposition, but neither a superposition of S nor of A and also not superposition of states of the composite system SA.

In $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$, S is in both states $|s_1\rangle$ and $|s_2\rangle$ simultaneously, as we know from the observed interference between 2 states.

However, in case of $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ experiment shows that SA is not in both two-part states $|s_1\rangle |a_1\rangle$ and $|s_2\rangle |a_2\rangle$ simultaneously, but only in two correlations simultaneously.

The entanglement of two systems is quite different from superposition of one system.

Experiments(Rarity et al) have demonstrated the precise sense in which $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ represents superposition.

Experiments answer question "given that S and A are in state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$, what (if any) entities interfere and what is nature of interference?"

22.5.2 Local State Solution of the Problem of Definite Outcomes

Consider a single quantum S(electron or photon), passing through double-slit experiment, with a "downstream" viewing screen.

Suppose an ideal "which-slit detector" A is present so that, upon detection, S and A become entangled in measurement state with orthogonal detection states $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$. Imagine S and A separated by meters or kilometers.

Complete observation of the experiment requires two "local observers", 1st observer is S and 2nd observer is A.

Such non-local setup has been carried out experimentally.

What did the local observers observe?

A well-known prediction of quantum physics says that first observer observes implications of "local state of S", represented by "reduced" density operator, where the degrees of freedom 2nd system are averaged over by the "trace" (Tr) operation (see derivation below)

$$\rho_{S} = \text{Tr}_{A}(\rho_{SA}) = |c_{1}|^{2} |s_{1}\rangle \langle s_{1}| + |c_{2}|^{2} |s_{2}\rangle \langle s_{2}|$$

and 2nd observer would observe implications of "local state of A", represented by the reduced density operator

$$\rho_A = \text{Tr}_S(\rho_{SA}) = |c_1|^2 |a_1\rangle \langle a_1| + |c_2|^2 |a_2\rangle \langle a_2|$$

where the density operator gives probabilities via the relation

$$P(q) = \operatorname{Tr}(\rho P_q) = \operatorname{Tr}(\rho |q\rangle \langle q|)$$

The "local state of S" is found by completely removing from the density operator any effects of A and vice versa. This is the important idea!

Derivation of reduced density operator

$$\rho_{SA} = |\psi_{SA}\rangle \langle \psi_{SA}| = (c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle) (c_1^* \langle s_1| \langle a_1| + c_2^* \langle s_2| \langle a_2|)$$

$$\rho_S = \operatorname{Tr}_A(\rho_{SA}) = \sum_{k=1}^2 \langle a_k| \rho_{SA} |a_k\rangle$$

$$= \sum_{k=1}^2 \langle a_k| (|\psi\rangle_{SA | SA} \langle \psi|) |a_k\rangle$$

$$= \sum_{k=1}^2 \langle a_k| ((c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle) (c_1^* \langle s_1| \langle a_1| + c_2^* \langle s_2| \langle a_2|)) |a_k\rangle$$

$$= \sum_{k=1}^2 (c_1 |s_1\rangle \delta_{k1} + c_2 |s_2\rangle \delta_{k2}) (c_1^* \langle s_1| \delta_{k1} + c_2^* \langle s_2| \delta_{k2})$$

$$= |c_1|^2 |s_1\rangle \langle s_1| + |c_2|^2 |s_2\rangle \langle s_2|$$
(22.61)

where we have used orthonormality via $\langle a_i | a_j \rangle = \delta_{ij}$. We note that the Tr (trace) operation = sum over all designated states removes all knowledge of designated system from equation. This is clearly useful if do not know much about reduced system. A similar derivation holds for ρ_A .

Continuing our discussion.

Reduced states are mixtures, not superpositions. QM predicts both LOCAL observers find mixtures not superpositions. Ensemble of experimental trials verifies this via mixed-state pattern in agreement with assertion made earlier

that neither S nor A is in a superposition.

For different example, $\rho_A = |c_1|^2 |a_1\rangle \langle a_1| + |c_2|^2 |a_2\rangle \langle a_2|$ predicts Schrödinger's cat is in mixture of either dead or alive, not superposition of both dead and alive.

The local states $\rho_S = \text{Tr}_A(\rho_{SA}) = |c_1|^2 |s_1\rangle \langle s_1| + |c_2|^2 |s_2\rangle \langle s_2|$ and $\rho_A = \text{Tr}_S(\rho_{SA}) = |c_1|^2 |a_1\rangle \langle a_1| + |c_2|^2 |a_2\rangle \langle a_2|$ must be taken seriously as implying the outcomes predicted to be observed at the two sites.

The local states cannot be dismissed simply by the argument that the only "real" state is "global state" $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$.

There is no contradiction between the predicted local mixtures $\rho_S = \text{Tr}_A(\rho_{SA}) = |c_1|^2 |s_1\rangle \langle s_1| + |c_2|^2 |s_2\rangle \langle s_2|$ and $\rho_A = \text{Tr}_S(\rho_{SA}) = |c_1|^2 |a_1\rangle \langle a_1| + |c_2|^2 |a_2\rangle \langle a_2|$ and the unitarily-evolving global pure state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$.

Important: To consider the combined system SA as single system only evolving unitarily misses the essential physics of nonlocality.

Haroche and Raimond weighed in on question of when a two-part system should be considered as a composite of two subsystems, versus when it should be considered single system B = SA.

The composite system should be considered a single system whenever the binding between the parts is much stronger than the interactions involved in the dynamics, so that internal structure of composite system is left unchanged as it travels through the experiment.

By this criterion, SA is not single system. Not only does the relation between S and A change during experiment, the relation is entangled and thus nonlocal.

The implication is that $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ must be considered an entanglement of two separate systems S and A, not superposition of a single composite system SA.

That's the basics of the theory! It follows completely from standard QM.

22.5.3 Now for even more details

Roch's "delayed choice" experiments used a Mach-Zehnder interferometer (Figure 22.4) rather than the logically equivalent double-slit setup, to observe photons.

As shown in detail in Figure 22.5, while a photon is on the 48-meter-long interferometer paths, a quantum-based random number generator "decided" whether the second beam splitter (positioned at the end of paths - note the spatial sepa-


Figure 22.4:



Figure 22.5:

ration) would be incorporated or omitted, i.e., it decided whether the detectors would not or would (respectively) determine "which path".

In trials incorporating the second beam splitter, an interference pattern is observed, indicating the photon passed as a superposition along both paths.

On trials omitting the second beam splitter, no interference is observed, indicating the photon passed as a mixture along one or the other path.

The two parallel paths were 5 millimeters apart.

Precisely (so far as the experiment could determine) when the second beamsplitter switched from "on" to "off", the photon changed in mid-flight from being on both paths to being on one or the other path.

The quantum jump was correlated with and coincident with the incorporation or the omission of the second beam splitter (i.e., with the decision to not entangle or to entangle the detectors with the photon).

All experimental results are just as predicted by the reduced states $\rho_S = \text{Tr}_A(\rho_{SA}) = |c_1|^2 |s_1\rangle \langle s_1| + |c_2|^2 |s_2\rangle \langle s_2|$ and $\rho_A = \text{Tr}_S(\rho_{SA}) = |c_1|^2 |a_1\rangle \langle a_1| + |c_2|^2 |a_2\rangle \langle a_2|$.

Switching the second beam-splitter off entangles the photon and the detector in the measurement state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ causing photon to collapse from superposition $|\psi\rangle_S = (c_1 |s_1\rangle + c_2 |s_2\rangle$ into the mixture $\rho_S = \text{Tr}_A(\rho_{SA}) = |c_1|^2 |s_1\rangle \langle s_1| + |c_2|^2 |s_2\rangle \langle s_2|$ that is observed at the detector.

At the diagonal density matrix stage, we are doing a classical measurement and it should be interpreted as such.

This resolves problem of definite outcomes!

Quantum theory predicts and experiment verifies that, with the detector in operation, observers of S and of A find them to be in definite mixtures, not indefinite superpositions!

Any strategy of imagining the quantum and the detector to be widely separated obviously changes nothing - it does not matter whether the quantum and the detector are close together or far apart.

The key to understanding quantum measurements comes from understanding the nonlocal relationship that develops between S and A when they evolve unitarily into entangled measurement state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$.

In experiments, global state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ violates Bell's inequality, implying an instantaneous non-local transfer of **correlations** across arbitrarily large distances. Without entanglement one would observe different results - the interferences would not disappear as in the experiments. But entanglement "decoheres-collapses" coherent states so that S and A impact their detectors randomly. Locally, entanglement decoheres each photon so that they exhibit definite outcomes.

But quantum dynamics is unitary, implying that the global state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ remains coherent despite the incoherence of subsystems.

Since the individual photons are now incoherently mixed, what has happened to coherence?

Answer: it is the experimentally observed global coincidence measurements

which compare the impact points of entangled pairs.

In a double-slit experiment with two screens, each photon "knows" the impact point (i.e., phase shift) of the other photon and instantly adjusts its own impact point in order to form an interference pattern as a function of the difference between the two photons' phase shifts!

This is strikingly non-local, and the experimental results violate Bell's inequality.

Thus the coherence of the entangled state resides in the correlations between subsystems, rather than in subsystems themselves!!

Entanglement transforms the coherence of states of S into coherence of correlations between states of S and A, allowing S and A to exhibit definite outcomes while preserving the global coherence as demanded by unitary evolution.

We can now answer the question: Precisely what is superposed and what interferes in measurement state?

The answer is surprisingly simple: Only the correlations between S and A are superposed. Thus the measurement state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ should be read as:

The state $|s_1\rangle$ is positively correlated with the state $|a_1\rangle$, and the state $|s_2\rangle$ is positively correlated with the state $|a_2\rangle$

Only correlations are superposed, not states.

When the superposition $|\psi\rangle_S = (c_1 |s_1\rangle + c_2 |s_2\rangle$ of S entangles with the states of A, the superposition shifts from a superposition of states of S to a superposition of correlations between S and A, so S can be in an incoherent mixture while maintaining unitary global dynamics!

This is how nature resolves problem of definite outcomes.

So the coherence exhibited by measurement state $|\psi\rangle_{SA} = c_1 |s_1\rangle |a_1\rangle + c_2 |s_2\rangle |a_2\rangle$ must be invisible to local observers, and yet show up in the global measurement state in order to preserve unitary dynamics.

One could regard this as the underlying reason why entanglement (i.e., measurement) must shift the coherence from the states of S and A to the correlations between S and A. "Collapse" can be viewed as consequence of measurement state's nonlocality plus special relativity's ban on instant signaling. We note that the global measurement state is a very different animal from local states. While the local mixed states are immediately observed at both local sites, the global state can be "observed" only **at some time after** measurement by traveling to both local sites, gathering data from both, and then assembling information and noting the correlations between two sets of data.

Another difficulty often raised in conjunction with measurement problem: "basis ambiguity" or "the preferred basis problem". The argument is that the local state solution based on reduced states is mathematically ambiguous in the special case that $|c_1|^2 = |c_2|^2 = 1/2$ because the reduced density operators become $\rho_S = I_S/2$ and $\rho_A = I_A/2$, where I_S and I_A are identity operators in the two reduced Hilbert spaces. Measurement does not determine a unique pair of subsystem basis vectors; any orthonormal basis can be used for each subsystem implying an ambiguous situation.

This is specious criticism because the measurement device is not constructed to pick out particular basis set in the subsystem's Hilbert space. It is designed instead to correlate with the particular physical state of measured quantum system. Regardless of what basis is used, the detector is designed to transition into $|a_i\rangle$ upon detecting S to be in $|s_i\rangle$, (i = 1, 2). It's not designed to transition into some other states such as $(|s_1\rangle+|s_2\rangle)/\sqrt{2}$. The particular physical states $|s_1\rangle$ and $|s_2\rangle$ determine, unambiguously, the "natural" basis of the measurement. In the double-slit experiment, these states are for example "quantum comes through slit 1" and "quantum comes through slit 2". The ambiguity of basis sets for the reduced density operators isn't important. What's important is the specific correlations established by detector!

Our conclusions so far:

When the detector measures the superposed quantum, quantum physics predicts that the states actually observed are local (i.e., mixed or reduced) states of subsystems, not the superposed global state that follows from Schrödinger's equation.

The local states directly observed in the measurement must contain no hint of nonlocal correlations between two subsystems since this would violate relativity's prohibition on instant signaling.

Thus the local states describe what actually happens at both subsystems.

The global state predicts these local states (can be derived from), and also predicts indirectly-observable (by gathering global data at later time) nonlocal correlations between these states.

22.5.4 An even more dramatic experiment

The unity of the quantum suggests that the measurement state (22.52) represents a unified, hence superposed and pure, quantum state of composite system. We asked the question: precisely what is superposed? We answered this question by studying the simple (i.e., non-composite) superposition (22.50) via interference exhibited in a Mach-Zehnder experiment.

Varying the lengths of either path 1 or path 2 created varying interference effects in detectors, demonstrating each photon really must travel both paths to its detector.

Quantum theory agrees entirely with these conclusions, as can be shown by using photon wavelengths to show that path differences correctly predict the interferences observed at each detector.

This implies that to understand the measurement state, one needs to find and analyze entanglement experiments that demonstrate interference. This has been done for several decades in connection with quantum non-locality. The key theoretical analysis was done by John Bell. Many nonlocal interference experiments have been done beginning with Clauser and Freedman culminating in experiments demonstrating nonlocality across great distances and that simultaneously closed all possible loopholes in all previous experiments.

By now, it is well known that the entangled state (22.52) predicts nonlocal effects between two subsystems, and that phase variations of either subsystem cause instantaneous, i.e., non-local, readjustments(correlations) of the possibly-distant other subsystem.

When macroscopic systems are involved (i.e., cats) we have a problem.

It is not easy to vary the phase of cat, and, as we saw in the Mach-Zehnder experiment, one cannot understand superposition without varying the phases of superposed parts.

Thus, all nonlocality experiments are carried out with pairs of simpler quanta such as photons.

The most recent nonlocal entanglement experiments most appropriate for investigating measurement were conducted nearly simultaneously by Rarity and Tapster and Ou. Figure 22.6 shows the layout for these "RTO" experiments.

The "source" creates entangled photon pairs by "parametric down-conversion". The RTO experiment is two back-to-back interferometer experiments but with first beam splitter for each photon located inside the source of entangled photons.

Without entanglement, each single photon (either A or B) would interfere with itself at own detectors according to own phase shift φ_A or φ_A .

Two entangled photons are emitted into a superposition of the solid paths con-



Figure 22.6:

necting detectors A1 and B1, and the dashed paths connecting detectors A2 and B2.

Note that the two photons are already entangled when emitted.

Entanglement changes everything.

No longer does either photon interfere with itself at its own detectors.

Instead, photons are entangled in measurement state (22.52) with $|\psi_1\rangle$ and $|\psi_2\rangle$ representing (say) the solid-line and the dashed-line states of A and $|1\rangle$ and $|2\rangle$ representing the solid-line and the dashed-line states of B, although in the RTO experiments neither subsystem is macroscopic.

Each photon now acts like which-path detector for other photon.

Recall the double-slit experiment:

When the which-slit detector is switched on, the pattern on screen switches abruptly from striped interference pattern indicating the pure state nature of each electron across both slits, to the phase-independent sum of two noninterfering single-slit patterns.

Entanglement between the electron and the which-slit detector breaks the pure state into two single-slit parts, so that the measured electron comes through either slit 1 or slit 2.

This suggests that in the RTO experiment, the entanglement should break the pure-state superposition into two non-interfering parts.

This is exactly what is observed. Both photons impact their detectors as random 50-50 mixtures, just like a flipped coin. Entanglement breaks the single-photon pure state (22.50) observed in the Mach-Zehnder experiment, causing each photon to behave "incoherently" with no dependence on its phase setting.

But (22.52) is pure state.

Where has phase dependence gone?

The answer lies in the phase-dependent but nonlocal relationship observed between the solid and the dashed branches. This phase dependence is observed experimentally in coincidence (or correlation) measurements comparing the detections of entangled pairs.

The "flipped coins" mentioned above turn out to be correlated with each other.

This phase dependence across two separated subsystems is essential to preserve the unity of the (now entangled) quantum.

This is not an easy experiment to perform:

The source creates a stream of photon pairs, and one must compare the impact of single photon A at detectors A1, A2 with the impact of corresponding entangled photon B at detectors B1, B2. RTO figured out how to do this, with the result shown in Figure 22.7.



Figure 22.7:

The figure graphs the degree of correlation between A and B. This is a measure of the agreement between the outcomes at A's detectors and B's detectors.

A correlation of +1 means perfect, or 100%, agreement: Either both sets of

detectors register outcome 1 (i.e., A1 and B1 click) or both register outcome 2.

The opposite extreme is a correlation of -1, meaning 100% disagreement: If one detector registers 1, the other registers 2.

Either correlation, +1 or -1, implies that either photon's outcome is predictable from the other photon's outcome.

A correlation of zero means one photon's outcome does not at all determine other's outcome: Each photon has random 50-50 chance of either outcome regardless of the other photon.

Correlations between 0 and +1 mean the outcomes are more likely to agree than to disagree, with larger correlations denoting higher probability of agreement; for example, correlation of +0.5 means 75% probability of agreement.

Similarly, correlations between 0 and -1 mean outcomes are more likely to disagree than to agree; a correlation of -0.5 means a 75% probability of disagreement.

The RTO experiment agrees entirely with predictions of standard quantum physics.

When accounting is made of the optical paths for both photons, they obtain the following result:

$$P(correlated) = P(A1 and B1) + P(A2 and B2) = \frac{1}{2} [1 + \cos(\varphi_B - \varphi_A)] (22.62)$$
$$P(anticorrelated) = P(A1 and B2) + P(A2 and B1) = \frac{1}{2} [1 - \cos(\varphi_B - \varphi_A)] (22.63)$$

where P(correlated) is a single-trial probability that A's and B's detectors will agree, and P(anticorrelated) is a single-trial probability that A's and B's detectors will disagree.

The degree of correlation, defined as P(correlated) - P(anticorrelated), is then simply $\cos(\varphi_B - \varphi_A)$, as graphed in Figure 7.

In 1964, John Bell published a ground-breaking article stating the sufficient condition for a statistical theory such as quantum physics to meet condition known as "locality". He defined locality to mean "that result of measurement on one system be unaffected by operations on distant system with which it has interacted in past".

Bell expressed a sufficient condition in form of inequality that any local theory must obey.

He demonstrated that certain statistical predictions of quantum physics violate Bell's inequality, i.e., quantum physics makes nonlocal predictions.

The results in Figure 7 implies the case in point: Figure 7 violates Bell's inequality at all phase differences $\varphi_B - \varphi_A$ other than 0, π , and 2π .

Let me underline meaning of this:

Violation of Bell's inequality means that the statistics of the measurements on photon A - photon A's "statistical behavior" - is necessarily affected by the setting of photon B's phase shifter.

In fact, even without Bell's condition, the nonlocality of the experiment intuitively obvious.

Here's why:

Suppose we set the phase shifters to zero and that all four optical paths (two solid, two dashed) are then equal; thus $\varphi_B - \varphi_A$ is zero.

Without the two beam splitters BS, the two photons emitted into the solid pair and the dashed pairs of paths would impact either detectors A1 and B1 or A2 and B2 because of symmetry of experiment and conservation of momentum. This is neither surprising nor nonlocal, and would happen even if the photons were not entangled.

But the beam splitter is a randomizing device that mixes the solid and dashed paths; any photon passing through it has a 50-50 chance of reflection or transmission.

With non-entangled photons and both beams splitters in place, there would then be no correlation between photon A's outcome and B's outcome because the two photons are independent of each other.

With entanglement, correlation is perfect.

How does one photon "know" which path the other photon took at the other photon's beam splitter?

Each photon is now "detecting" the quantum state of the other photon, from a distance that could be large.

Perfect correlation certainly "feels" nonlocal even though (as mentioned above) this perfect correlation at $\varphi_B - \varphi_A = 0$ does not violate Bell's inequality. Note that such a violation is a sufficient but not a necessary condition for nonlocality.

Non-locality is written all over the RTO experiment.

Each photon "knows" which direction the other photon takes at its beam splitter and adjusts its selection accordingly.

The key nonlocal feature of graph, which is simply a cosine function, has $(\varphi_B - \varphi_A)$ as its independent variable. Thus any desired shift in correlations can be made by an observer at either of possibly-widely-separated phase shifters.

Bell suspected that this situation meant that observer A (call her Alice) could use her phase shifter to alter outcomes that would have occurred at both her own and observer B's (call him Bob) detector and, following up on this hypothesis, derived his inequality involving probabilities at both Alice's and Bob's detectors which, if violated, implied that both photons must have readjusted their states.

Such a readjustment is just what we expect, given the unity of quantum and thus the unity of atoms and other entangled systems such as our two photons.

Two photons form a single "bi-quantum", an "atom of light", in the pure state (22.52).

When Alice varies her phase shifter, both photons "know" both path lengths and readjust their behavior accordingly to produce the proper correlations.

Analogously, a single photon "knows" both path lengths in single-photon interferometer experiment.

Finally, we come to the central question of the discussion:

What is actually superposed in entangled superposition (22.52)?

A Mach-Zehnder experiment tests the simple superposition (22.50), while the RTO experiment tests the entangled superposition (22.52).

We know what is superposed in Mach-Zehnder, namely quantum states $|\psi_1\rangle$ (path 1) and $|\psi_2\rangle$ (path 2). This is deduced from the effect that either phase shifter has on both states.

Now consider the RTO experiment. What is the effect of shifting either phase shifter?

One thing that does not change is the state ("local state" would be a better term, as discussed earlier) of either photon A or photon B:

As we know, both photons remain in 50-50 mixtures regardless of either phase setting.

What does change with variations in either phase shifter is the correlations between A and B.

With $\varphi_B - \varphi_A = 0$ we have perfect correlation: Either A1 and B1 (which we denote (11)) or A2 and B2 (denoted (22)).

As we vary either φ_B or φ_A we obtain non-zero probabilities of anti-correlated individual trials, denoted (12) (outcomes A1 and B2) and (21) (A2 and B1).

When non-local phase angle difference $(\varphi_B - \varphi_A)$ reaches $2\pi/2$, we have zero correlation, and when it eaches π have perfect anti-correlation.

Table 1 summarizes the crucial points in more detail.

The column titled "simple superposition" shows how the superposition state of single photon (M-Z) varies from "100% state 1" to "100% state 2" as the phase angle between two states varies.

The column titled "entangled superposition of two subsystems" shows that the state of each photon remains unchanged throughout the entire range of both phase settings, while the nonlocal correlation between states of two photons varies from "100% correlated" to "zero correlation" and then to "100% anticorrelated" as either of the two local phase angles varies.

| Simple superposition: | | Entangled superposition of two sub-systems: | | |
|-----------------------|------------------|---|----------------------|---------------------|
| φ - | State of photon | $\varphi_{\rm B}$ - $\varphi_{\rm A}$ | State of each photon | Correlation between |
| | | · · | • | the two photons |
| 0 | 100% "1", 0% "2" | 0 | 50-50 "1" or "2" | 100% corr, 0% anti |
| π/4 | 71% "1", 29% "2" | π/4 | 50-50 "1" or "2" | 71% corr, 29% anti |
| π/2 | 50% "1", 50% "2" | π/2 | 50-50 "1" or "2" | 50% corr, 50% anti |
| $3\pi/4$ | 29% "1", 71% "2" | $3\pi/4$ | 50-50 "1" or "2" | 29% corr, 71% anti |
| π | 0% "1", 100% "2" | π | 50-50 "1" or "2" | 0% corr, 100% anti |

Table 1. In a simple superposition, the photon's state varies with phase angle. In an entangled superposition, the relationship between states of the two photons varies, while individual states of both photons are phase-independent (or "mixed").

So once again, what is superposed in RTO experiment?

The hallmark of a superposition is the dependence on phase difference between the objects superposed.

But Table 1 exhibits no such phase dependence of states of two photons.

Each photon remains in unchanging 50-50 mixture of their own "path 1" and "path 2" states - a situation that is radically at odds with the true superposition of path 1 and path 2 exhibited by M-Z experiment.

Thus, in the entangled RTO state, neither photon is superposed.

We see here the source of the "classical" or non-superposed nature of reduced density operators (22.57) and (22.58)), not to mention the non-superposed and hence non-paradoxical nature of Schrödinger's cat.

Examination of the phase-dependence of the measurement state (22.52), as demonstrated by nonlocality experiments such as RTO experiment, reveals the true nature of Schrödinger's cat. The last column of Table 1 shows us what actually is superposed when two subsystems are entangled in measurement state (22.52).

Since the correlations between two photons vary sinusoidally as the non-local phase angle between the two photons varies, clearly these are correlations between the states of two photons, and not the states themselves, that are interfering.

Entanglement has shifted superposition, from states of one photon A ((22.50), M-Z) to correlations between photon A and photon B ((22.52), RTO).

More Details and Conclusions

In order to resolve problem of definite outcomes of measurements, aka Schrödinger's cat, the discussion analyzes the entangled state (22.52) of a microscopic quantum and its macroscopic measuring apparatus.

This state is a superposition of two composite entities $|\psi_1\rangle|1\rangle$ and $|\psi_2\rangle|2\rangle$, with a phase angle between these entities that can range over 2π radians.

In the measurement, this phase angle is fixed at zero because they designed the detector so that the two basis states of measured quantum are 100% positively correlated with the basis states of measurement apparatus.

To resolve problem of definite outcomes we must ask(as we have already done several times):

Precisely what does the composite superposition (22.52) actually superpose, physically?

In order to understand a simple non-composite superposition (22.50), we looked at the effect of varying the phase angle between superposed entities $|\psi_1\rangle$ and $|\psi_2\rangle$ in experimental setting such as M-Z interferometer.

The theoretically predicted and experimentally observed results then made it obvious that the quantum whose state is (22.50) flows simultaneously along two separate paths described by $|\psi_1\rangle$ and $|\psi_2\rangle$.

To understand the superposition (22.52), one should proceed similarly by studying situations in which phase angle between superposed entities $|\psi_1\rangle|1\rangle$ and $|\psi_2\rangle|2\rangle$ varies.

One lesson of this analysis is that, in order to understand the measurement problem, one must understand the significance of nonlocality.

This is because the key measurement state (22.52) that caused Schrödinger and decades of experts so much concern has nonlocal characteristics.

It must be understood as a superposition of correlations, rather than a superposition of states, but this cannot become apparent until one considers the effect of variations in phase angle between its superposed terms.

Such variations are not part of the measurement process itself because measurements are designed to take place at zero phase angle.

Experimental or theoretical studies of such phase variations will have nonlocal ramifications, because such variations are inherently nonlocal!!

It's worth emphasizing that, when two subsystems are entangled in measurement state (22.52), neither subsystem is superposed - only the correlations between subsystems are superposed.

In RTO experiments, the two correlations in question are represented by the solid and the dashed paths connecting pairs of outcomes. A pair of photons entangled in state (22.52) follows both of these paths simultaneously.

The subsystems themselves, however, are not in superpositions but instead in indeterminate mixtures of definite states. Thus observers of either subsystem will observe only definite outcomes, as predicted by the local mixtures (22.57) and (22.58).

RTO experiments are the entangled analog of the M-Z interferometer experiment: a pair of back-to-back interferometer experiments, with entangled pair of quanta of which one quantum passes through each interferometer.

As we said earlier, the experiment and its theoretical analysis shows that, when a superposed photon A becomes entangled with second photon B to form state (22.52), the nonlocal aspect of A's superposition is transferred to the correlations between A and B.

Thus, an entangled state such as (22.52) is neither a superposition of states of A nor of states of B, but instead superposition of correlations between states of A and states of B.

To see this most clearly, we compare the simple superposition (22.50) with the entangled superposition (22.52).

In the simple superposition, the state observed by a "which-state" detector varies smoothly from 100% $|\psi_1\rangle$, through 50% $|\psi_1\rangle$ and 50% $|\psi_2\rangle$, and finally to 100% $|\psi_1\rangle$ as the phase angle φ between $|\psi_1\rangle$ and $|\psi_2\rangle$ varies from 0 to π .

In the entangled superposition, neither the state of A nor the state of B varies as φ_A or φ_B varies; both A and B remain in 50-50 mixtures throughout. What does vary is the correlation between A and B.

A non-local "correlation detector" (i.e., an RTO-type of experiment!) would find relation between the two subsystems varies from 100% positively correlated (either pair state 11 or 22, pictured by solid and dashed paths in Figure 6), to 50% positively correlated and 50% anti-correlated, and finally to 100% anticorrelated (12 or 21), as the nonlocal phase difference $\varphi_B - \varphi_A$ varies from 0 to π .

This is a superposition of correlations, not a superposition of composite states or of non-composite (single-system) states.

At least in the idealized case of a minimally-disturbing von Neumann measurement, the initial stage of measurement process (through formation of measurement state (22.52)) can be described as follows:

A quantum in a simple superposition such as (22.50) entangles with a macroscopic which-path detector.

At the instant of entanglement, the local states of both the quantum and the detector undergo a radical change, a quantum jump.

Locally, the detector and the quantum jump into mixtures (22.57) and (22.58).

Simultaneously, the global state (22.52) continues evolving smoothly according to Schrödinger equation.

Entanglement causes the superposed single quantum to be instantly transformed into superposed correlations between the quantum and the detector.

This stage of measurement process is entirely describable in terms of a pure global states following Schrödinger equation.

"Collapse" from the local superposition to the local mixtures occurs because of the formation of the entangled state (22.52) and the resulting formation of subsystems whose local states ((22.57) and (22.58)) have definite outcomes. Note that the phenomenon of nonlocality is essential to preserving the purestate nature (the unity) of the composite system.

To put this more intuitively, a reorganization throughout the entire extent of the composite entangled system is required in order to preserve the unity of the (now entangled) quantum.

According to Table 1, when two systems entangle to form the state (22.52), both "collapse" into phase-independent local mixtures.

Relativity requires this phase independence:

If any phase-dependent aspect of entangled state were locally observable, instant information-containing messages could be sent, violating special relativity. Local states of entangled subsystems must be invariant to phase changes.

Thus, only the relationship - the correlations - between A and B, but not A or B themselves, can vary with phase angle. Since local observers cannot detect these correlations, the entangled state cannot be used to send superluminal signals.

This is, ultimately, the reason Schrödinger's cat must be either alive or dead rather than superposition of both. A phase-dependent superposition involving both local states would permit nonlocal signaling, violating relativity.

This conclusion implies that standard physical description of composite nonentangled (i.e., factorable) product state such as $|\psi_1\rangle|1\rangle$ has been long mistaken.

Usually we regard $|\psi_1\rangle|1\rangle$ as state of the composite system AB, where subsystem A is in state $|\psi_1\rangle$ and subsystem B is in state $|1\rangle$. But this leads us into the paradox of Schrödinger's cat, where (22.52) represents a state in which two macroscopically different composite states exist simultaneously as a superposition.

According to present discussion, quantum theory and quantum experiments imply this entangled state to be a superposition of correlations between states rather than a superposition of composite states.

Thus $|\psi_1\rangle|1\rangle$ is not a state of composite system, but instead a correlation between two subsystems. That is, $|\psi_1\rangle|1\rangle$ means "subsystem A is in state $|\psi_1\rangle$ if and only if subsystem B is in state $|1\rangle$ ", an important departure from usual description.

Even if one of two subsystems happens to be a macroscopic detector, the entangled state (22.52) is simply a non-paradoxical superposition of correlations. It says merely that state $|\psi_1\rangle$ of A is correlated with state $|1\rangle$ of B, and state $|\psi_2\rangle$ of A is correlated with the state $|2\rangle$ of B, with non-local phase angle $\varphi_B - \varphi_A$ determining the degree of each correlation.

In the case of a measurement, this phase angle is fixed at zero.

Regardless of the phase angle, neither subsystem is in superposition.

The entangled measurement state (22.52) is best described as a "macroscopic correlation": a pair of superposed (i.e., phase-dependent) quantum correlations in which one subsystem happens to be macroscopic. It is technically very difficult to create a macroscopic superposition, but macroscopic which-path detectors routinely achieve the state (22.52). It's not paradoxical, even though many analyses have puzzled over it.

In entanglement, nature employs an ingenious tactic. She must not violate relativistic causality, yet she must be nonlocal in order to maintain the pure-state nature of original single-quantum superposition over composite objects such as bi-photons.

Thus, she accomplishes nonlocality entirely via the superposition of correlations, because correlations cannot be locally detected and thus their superposition cannot violate relativity. This tactic lies behind the nonlocal spread of phasedependence over large spatial distances.

By means of the superposition of correlations - entanglement - nature creates a phase-dependent pure-state quantum structure across extended quantum systems such as bi-photons.

I've frequently used the term "local" as contrasted with "global". For composite systems, and especially the entangled measurement state, it's a crucial distinction.

Entangled states such as (22.52) have distinct local and global (nonlocal) aspects.

The local description corresponds to two observers, each observing only one subsystem. In the case of (22.52), this "local description" is fully captured by the reduced density operators (22.57) and (22.58) - each local observer detects a mixture, not a superposition, of one subsystem.

The "global description" means the evolving pure state of the entire composite system, in our case (22.52). It is a superposition of nonlocal correlations that can only be detected by observing both subsystems and, via an ensemble of trials that individually record corresponding outcomes at both subsystems, determining the state of the correlations between them.

Although the global state implies the local description, the local description

cannot hint at the global correlations because any such hint would violate Einstein causality.

Thus, when an electron shows up in your lab, neither an examination of the electron nor an examination of an ensemble of identically-created electrons can give you the least hint of whether or how this electron is entangled with other quanta elsewhere in the universe.

This clarification of entanglement resolves problem of definite outcomes, aka Schrödinger's cat.

An ideal measurement of a superposed microscopic system A by a macroscopic detector B establishes the measurement state (22.52) at 100% positive correlation. This state is equivalent to the logical conjunction "A is in local state $|\psi_1\rangle$ if and only if B is in local state $|1\rangle$, AND A is in local state $|\psi_2\rangle$ if and only if B is in local state $|1\rangle$ ", where AND indicates the superposition. This conjunction is precisely what we want following a measurement.

Schrödinger's cat is not in the least paradoxical.

This analysis does not entirely resolve the quantum measurement problem.

It resolves the problem of definite outcomes associated with the measurement state (22.52), but this state continues to obey Schrödinger's equation and, hence, is reversible.

In fact, the entangled state between a quantum and its which-path detector can actually be reversed in the Stern-Gerlach experiment.

In my view, a quantum measurement must result in a macroscopic indication such as a recorded mark, and a mark is irreversible.

The above analysis shows the entangled state (22.52) describes a mixture of definite, not superposed, outcomes of measurements, but these outcomes remain indeterminate and the global state remains reversible.

The irreversibility problem is the question of how this nonlocal superposition of correlations then further "collapses" irreversibly to just one of its possible outcomes, a "collapse" that occurs in the RTO experiment only when one photon impacts a detector.

The present analysis does not seem to resolve this problem.

In the case of the RTO experiment, however, it seems fairly clear that the nonlocal superposition described by Eq. (22.52) must irreversibly decohere(register a value) when either of its subsystems A or B interacts with a detector. The RTO experiment furnishes a particularly good setting for this question, because the two photons remain in the reversible entangled state (22.52) throughout their flights from the source to detectors, and thus the two key questions of the measurement problem (the problem of definite outcomes and the problem of irreversibility) can be analyzed individually.

22.6 Closing Story #1

Let us look at EPR again now that we understand what is happening in entangled quantum systems.

Depending on basis used (language chosen) we have one of two states for a pair of electrons:

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle |\downarrow_z\rangle - |\downarrow_z\rangle |\uparrow_z\rangle) \quad \text{or} \quad |\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow_x\rangle |\downarrow_x\rangle - |\downarrow_x\rangle |\uparrow_x\rangle) \tag{22.64}$$

Let us once again consider the EPR reasoning to see whether it leads to the conclusion of incompleteness of quantum mechanics. If Alice performs a measurement on spin along the z direction and the outcome is spin up, the state vector after measurement is updated to $|\uparrow_z\rangle|\downarrow_z\rangle$.

This just means that if Bob were to measure the *z*-component of spin, the spin value would be DOWN according to Alice. This description of physical reality is true only **relative to Alice**.

From Bob's perspective, before he knows the Alice's measurement result, he still views the composite system in the original state, i.e., no quantum event happened yet. In other words, Bob still predicts that future measurement spin will find the UP state with fifty percentage of chance.

Since the spins of the two electrons are entangled, Alice's spin is a measuring apparatus for Bob's spin.

Since Alice performed a spin measurement, she effectively reads the measuring apparatus. Therefore, she is the intrinsic observer, and Bob is an external observer. At this point, both observers are out of synchronization on the relational information of the two particles, thus they give different predictions of the Bob particle spin value.

To verify the physical description Alice obtained for the Bob spin value after measuring the Alice particle spin value, Alice can travel to Bob's location to perform a measurement, or can send the measurement result to Bob and ask Bob to perform a measurement.

Suppose Alice sends the measurement outcome to Bob. Bob updates state to

 $|\uparrow_z\rangle|\downarrow_z\rangle$, the same as state relative to Alice.

He now can confirm the physical reality that the Bob spin value is DOWN with unit probability.

However, in this state, he cannot predict deterministically that Bob particle spin value is would be in the x-direction, since $|\downarrow_z\rangle$ is superposition of x-components.

Similarly, if Alice performs a measurement on the Alice particle spin along the x-direction and the outcome is spin UP, then the Bob particle spin value is deterministically DOWN(x-direction) relative to Alice, but nothing happened from Bob's view.

If Alice sends the measurement result to Bob, Bob updates the state vector accordingly to $|\uparrow_x\rangle|\downarrow_x\rangle$. He now can confirm the physical reality that the Bob particle spin value is the right state $|\downarrow_x\rangle$.

However, in this state, he cannot predict deterministically that the Bob particle spin value would be in the z-direction, since $|\downarrow_x\rangle$ is superposition of z-components.

Since Alice cannot perform measurement on the Alice spin value along z and x directions at the same time, Bob cannot confirm the Bob spin value has spin values in both z and x directions simultaneously. The reality that the Bob spin value simultaneously have definite values for S_z and S_x cannot be verified.

This is consistent with the Heisenberg Uncertainty Principle. There is no incompleteness issue for quantum mechanics. Hence the original EPR argument.

However, there is still a puzzle here, namely, a non-causal correlation.

It appears Bob's measurement outcome on the Bob spin value "depends" on which direction Alice chooses to measure the Alice spin value.

Since Alice's measurement does not impact the physical property of particle Bob spin value, we can ask exactly what spin state is Bob spin value in before Alice's measurement?

To answer this subtle question, first note that it is Alice's new knowledge of the Bob spin value, not the physical reality of the Bob spin value, that depends on the axis along which the measurement is performed.

One cannot assume there exists an absolute reality for Bob spin value.

To confirm the new found reality of the Bob spin value relative to Alice, Alice sends the measurement result to Bob who performs a subsequent measurement.

There is no faster-than-light action here.

Secondly, it is true that Bob's measurement outcome correlates to the Alice's measurement result. But this is an informational correlation, not a causal relation.

This correlation is encoded in the entangled state of the composite system $|\psi\rangle$. Since the entanglement is preserved even when both particles are space-like separated, the correlation is preserved.

Such an entangled quantum state contains not only the classical correlation, but also the coherence information of the composite system.

When Alice measures the Alice particle spin value, she effectively measures the composite system, because she obtains information not only about the Alice spin value, but also about the correlation between the Alice spin value and the Bob spin value.

In addition, the measurement induces the decoherence of the composite system.

Before Alice performs the measurement, it is meaningless to speculate what spin state the Bob particle spin is in.

When Alice measures the Alice spin value along the z direction and obtains result of spin up, she knows that in this condition, the Bob spin value is in spin down and later this is confirmed by Bob.

If instead, she measures the Alice spin value along the x direction and obtains result of spin left, she knows that in this new condition, the Bob spin value is in spin right and is later confirmed by Bob.

To better understand this non-causal relation, suppose we have many identical copies of the entangled pairs described by $|\psi\rangle$.

Alice measures the Alice particle spin values sequentially along the z direction and she does not send measurement results to Bob. Bob independently measures the Bob particle spin values along z direction as well.

Both of them observe their own measurement results for S_z as randomly spin up or spin down, but with fifty percent of chance for each. When later they meet, compare measurement results. They find two sequences of S_z values that are exactly opposite.

They can even choose a random sequence of z or x directions but both follow exact sequence in their independent measurements. When later they meet and compare measurement results, they still find their measured values are the opposite sequentially.

What does this all mean?

Special Relativity forces us to abandon the concept of absolute time.

Measurement of time is observer-dependent.

Similarly, in relativistic QM, the idea of an observer independent quantum state must be abandoned.

Space-like separated observers, however, can reconcile the different descriptions of the same quantum system through classical communication of information obtained from local measurements.

22.7 Closing Story #2 - Some Provocative Thoughts

Quantum mechanics began with Heisenberg's "Umdeutung(Reinterpretation)" paper, i.e., his proposed "reinterpretation" of physical quantities at the fundamental level as non-commutative.

To say that the algebra of physical quantities is commutative is equivalent to saying that the projection operators form a Boolean algebra (Boolean algebra is the branch of algebra in which the values of the variables are the truth values true and false, usually denoted 1 and 0 respectively).

They represent yes-no observables, or properties (for example, the property that the energy of the system lies in a certain range of values), or propositions (the proposition asserting that the value of the energy lies in this range), with the two eigenvalues corresponding to the truth values, true and false.

Heisenberg's insight amounts to the proposal that certain phenomena in our Boolean macroworld that defy a classical physical explanation can be explained probabilistically as a manifestation of collective behavior at a non-Boolean micro-level.

The Boolean algebra of physical properties of classical mechanics is replaced by a family of "intertwined" Boolean algebras, one for each set of commuting observables.

The intertwinement precludes the possibility of embedding the whole collection into one inclusive Boolean algebra, so you can't assign truth values consistently to the propositions about observable values in all these Boolean algebras.

Putting it differently: there are Boolean algebras in the family of Boolean alge-

bras of a quantum system, notably the Boolean algebras for position and momentum, or for spin components in different directions, that don't fit together into a single Boolean algebra, unlike the corresponding family for a classical system.

The intertwinement of commuting and noncommuting observables in Hilbert space imposes objective pre-dynamic probabilistic constraints on correlations between events.

The probabilistic constraints encoded in the geometry of Hilbert space provide the framework for the physics of a genuinely indeterministic universe.

They characterize the way probabilities fit together in a world in which there are nonlocal probabilistic correlations that violate Bell's inequality.

Quantum probabilities don't quantify incomplete knowledge about a state, but reflect the irreducibly probabilistic relation between the non-Boolean microlevel and the Boolean macrolevel.

This means that quantum mechanics is quite unlike any theory we have dealt with before in the history of physics, and there is no reason, apart from tradition, to assume that the theory can provide the sort of explanation we are familiar with in a theory that is commutative or Boolean at the fundamental level.

Quantum probabilities can't be understood in the Boolean sense as quantifying ignorance about the pre-measurement value of an observable, but give results in terms of what you'll find if you "measure", which involves considering the outcome, at the Boolean macrolevel, of manipulating a quantum system in a certain way.

A quantum "measurement" is a bit of a misnomer and not really the same sort of thing as a measurement of a physical quantity of a classical system.

It involves putting a microsystem, like a photon, in a situation, say a beamsplitter or an analyzing filter, where the photon is forced to make an intrinsically random transition recorded as one of two macroscopically distinct alternatives in a device like a photon detector.

The registration of the measurement outcome at the Boolean macrolevel is crucial, because it is only with respect to a suitable structure of alternative possibilities that it makes sense to talk about an event as definitely occurring or not occurring, and this structure is a Boolean algebra.

From this perspective, Heisenberg's theory provides a way of deriving probabilities and probabilistic correlations with no causal explanation. They are "uniquely given from the start" as a feature of the non-Boolean structure, related to the angles in Hilbert space, not measures over states as they are in a classical or Boolean theory.

The really significant thing about a noncommutative mechanics is the novel possibility of correlated events that are intrinsically random, not merely apparently random like coin tosses, where the probabilities of "heads" and "tails" represent an averaging over differences among individual coin tosses that we don't keep track of for practical reasons.

This intrinsic randomness allows new sorts of nonlocal probabilistic correlations for "entangled" quantum states of separated systems.

The view that Hilbert space is fundamentally a theory of probabilistic correlations that are structurally different from correlations that arise in Boolean theories is, in effect, an information-theoretic interpretation of quantum mechanics.

On this way of understanding quantum mechanics, as a non-classical theory of information or a new way of generating probabilities and probabilistic correlations between intrinsically random events, probabilities are defined with respect to a single Boolean frame, the Boolean algebra generated by the "pointerreadings" - the "ultimate measuring instruments", which are "kept outside the system subject to quantum mechanical treatment"

It's not that unitarity is suppressed at a certain level of complexity, where non-Booleanity becomes Booleanity and quantum becomes classical.

Rather, there is a macrolevel, which is Boolean, and there are actual events at the macrolevel.

Any system, of any complexity, is fundamentally a quantum system and can be treated as such, in principle, which is to say that a unitary dynamical analysis can be applied to whatever level of precision you like.

The crucial assumption in this probabilistic interpretation of the theory is that the outcome of a measurement is an intrinsically random event at the macrolevel, something that actually happens, not described by the deterministic unitary dynamics, so outside the theory, or "irrational".

Putting it differently, the "collapse", as a conditionalization of the quantum state, is something you put in by hand after recording the actual outcome.

The physics doesn't give it to you.

Special relativity, as a theory about the structure of space-time, provides an

explanation for length contraction and time dilation through the geometry of Minkowski space-time, but that's as far as it goes.

This explanation didn't satisfy Lorentz, who wanted a dynamical explanation in terms of forces acting on physical systems used as rods and clocks.

Quantum mechanics, as a theory about randomness and nonlocality, provides an explanation for probabilistic constraints on events through the geometry of Hilbert space, but that's as far as it goes.

22.8 Last Thoughts

When a detector measures a superposed quantum, quantum physics predicts that states actually observed are local (i.e., mixed or reduced) states of subsystems, not the superposed global state that follows from Schrödinger's equation. The local states that are directly observed in a measurement must contain no hint of the nonlocal correlations between the two subsystems, lest relativity's prohibition on instant signaling be violated.

Thus the local states describe what actually happens in both subsystems.

The global state predicts these local states, and also predicts the indirectlyobservable (by gathering global data at a later time) nonlocal correlations between these states.

Experiments confirm both the local and the global predictions, namely that outcomes are definite but unpredictable, and correlations between these definite outcomes are as described by the entangled measurement state.

This resolves problem of definite outcomes of measurements.

Nonlocality experiments demonstrate the precise nature of superposition inherent in the global measurement state:

This state is a superposition only of correlations between the detector and its observed quantum, not a superposition of states of the detector or quantum. It should be read as "first the quantum state is correlated with the first detector state AND the second quantum state is correlated with the second detector state".

The word AND indicates superposition. By this shifting of coherence from states of subsystems to correlations between subsystems that evolution of global state can remain unitary, and global state can remain coherent, while both subsystems collapse into incoherent mixtures of unpredictable but definite outcomes. This is the way nature resolves problem of definite outcomes. Analyses such as this are sometimes called "no-collapse" solutions of measurement problem, but this is a misnomer. There is a physically real, instantaneous, and observable collapse - a quantum jump- of observed local states, as verified quite explicitly by Roch's delayed-choice experiment.

The global state cannot collapse because it obeys unitary dynamics; it accordingly entangles rather than collapses upon measurement. Observed phenomena collapse, while the global state continues smoothly evolving as predicted by Schrödinger's equation.

The notion of "collapse of the quantum state" must be replaced by "collapse of the local state, and unitary evolution of the global state".

Both aspects, local and global, are correctly predicted by standard quantum theory and verified by experiments.

There is no problem with standard quantum mechanics!