Quantum Mechanics

Mathematical Structure
and
Physical Structure

Problems

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Contents

Chapter 3

Formulation of Wave Mechanics - Part 2

3.11 Problems

3.11.1 Free Particle in One-Dimension - Wave Functions

Consider a free particle in one-dimension. Let

$$\psi(x,0) = N e^{-\frac{(x-x_0)^2}{4\sigma^2}} e^{i\frac{p_0 x}{\hbar}}$$

where x_0, p_0 and σ are real constants and N is a normalization constant.

(a) Find $\tilde{\psi}(p,0)$

(b) Find $\tilde{\psi}(p,t)$

(c) Find $\psi(x,t)$

(d) Show that the *spread* in the spatial probability distribution

$$\wp(x,t) = \frac{|\psi(x,t)|^2}{\langle \psi(t) \mid \psi(t) \rangle}$$

increases with time.

3.11.2 Free Particle in One-Dimension - Expectation Values

For a free particle in one-dimension

$$H = \frac{p^2}{2m}$$

(a) Show $\langle p_x \rangle = \langle p_x \rangle_{t=0}$

(b) Show $\langle x \rangle = \left[\frac{\langle p_x \rangle_{t=0}}{m}\right] t + \langle x \rangle_{t=0}$

(c) Show $(\Delta p_x)^2 = (\Delta p_x)^2_{t=0}$

(d) Find $(\Delta x)^2$ as a function of time and initial conditions. HINT: Find

$$\frac{d}{dt}\left\langle x^2\right\rangle$$

To solve the resulting differential equation, one needs to know the time dependence of $\langle xp_x + p_x x\rangle$. Find this by considering

$$\frac{d}{dt}\left\langle xp_x + p_x x\right\rangle$$

3.11.3 Time Dependence

Given

$$H\psi = i\hbar\frac{\partial\psi}{\partial t}$$

with

$$H = \frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x})$$

(a) Show that $\frac{d}{dt}\langle\psi(t) \mid \psi(t)\rangle = 0$

(b) Show that $\frac{d}{dt}\langle x\rangle = \left\langle\frac{p_x}{m}\right\rangle$

(c) Show that $\frac{d}{dt}\langle p_x\rangle = \left\langle -\frac{\partial V}{\partial x}\right\rangle$

(d) Find $\frac{d}{dt}\langle H\rangle$

(e) Find $\frac{d}{dt}\langle L_z\rangle$ and compare with the corresponding classical equation $\left(\vec{L} = \vec{x}\times\vec{p}\right)$

3.11.4 Continuous Probability

If $p(x) = xe^{-x/\lambda}$ is the probability density function over the interval $0 < x < \infty$, find the mean, standard deviation and most probable value(where probability density is maximum) of x.

3.11.5 Square Wave Packet

Consider a free particle, initially with a well-defined momentum p_0, whose wave function is well approximated by a plane wave. At $t = 0$, the particle is localized in a region $-a/2 \le x \le a/2$, so that its wave function is

$$\psi(x) = \begin{cases} Ae^{ip_0x/\hbar} & -a/2 \le x \le a/2 \\ 0 & \text{otherwise} \end{cases}$$

(a) Find the normalization constant A and sketch $\mathrm{Re}(\psi(x))$, $\mathrm{Im}(\psi(x))$ and $|\psi(x)|^2$

(b) Find the momentum space wave function $\tilde{\psi}(p)$ and show that it too is normalized.

(c) Find the uncertainties Δx and Δp at this time. How close is this to the minimum uncertainty wave function.

3.11.6 Uncertain Dart

A dart of mass $1\,kg$ is dropped from a height of $1\,m$, with the intention to hit a certain point on the ground. Estimate the limitation set by the uncertainty principle of the accuracy that can be achieved.

3.11.7 Find the Potential and the Energy

Suppose that the wave function of a (spinless) particle of mass m is

$$\psi(r,\theta,\phi) = A\frac{e^{-\alpha r} - e^{-\beta r}}{r}$$

where A, α and β are constants such that $0 < \alpha < \beta$. Find the potential $V(r,\theta,\phi)$ and the energy E of the particle.

3.11.8 Harmonic Oscillator wave Function

In a harmonic oscillator a particle of mass m and frequency ω is subject to a parabolic potential $V(x) = m\omega^2 x^2/2$. One of the energy eigenstates is $u_n(x) = Axexp(-x^2/x_0^2)$, as sketched below.

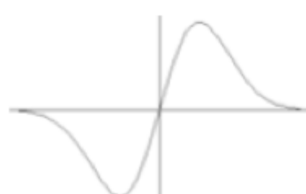

Figure 3.1: A Wave Function

(a) Is this the ground state, the first excited state, second excited state, or third?

(b) Is this an eigenstate of parity?

(c) Write an integral expression for the constant A that makes $u_n(x)$ a normalized state. Evaluate the integral.

3.11.9 Spreading of a Wave Packet

A localized wave packet in free space will spread due to its initial distribution of momenta. This wave phenomenon is known as *dispersion*, arising because the relation between frequency ω and wavenumber k is not linear. Let us look at this in detail.

Consider a general wave packet in free space at time $t = 0$, $\psi(x, 0)$.

(a) Show that the wave function at a later time is

$$\psi(x,t) = \int_{-\infty}^{\infty} dx'\, K(x,x';t)\psi(x')$$

where

$$K(x,x';t) = \sqrt{\frac{m}{2\pi i\hbar t}} exp\left[\frac{im(x-x')^2}{2\hbar t}\right]$$

is known as the *propagator*. [HINT: Solve the initial value problem in the usual way - Decompose $\psi(x, 0)$ into stationary states (here plane waves), add the time dependence and then re-superpose].

(b) Suppose the initial wave packet is a Gaussian

$$\psi(x,0) = \frac{1}{(2\pi a^2)^{1/4}} e^{ik_0 x} e^{-x^2/4a^2}$$

Show that it is normalized.

(c) Given the characteristic width a, find the characteristic momentum p_c, energy E_c and the time scale t_c associated with the packet. The time t_c sets the scale at which the packet will spread. Find this for a macroscopic object of mass $1\, g$ and width $a = 1\, cm$. Comment.

(d) Show that the wave packet probability density remains Gaussian with the solution

$$P(x,t) = |\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi a(t)^2}} exp\left[-\frac{(x-\hbar k_0/m)^2}{2a(t)^2}\right]$$

with $a(t) = a\sqrt{1 + t^2/t_c^2}$.

3.11.10 The Uncertainty Principle says ...

Show that, for the 1-dimensional wavefunction

$$\psi(x) = \begin{cases} (2a)^{-1/2} & |x| < a \\ 0 & |x| > a \end{cases}$$

the rms uncertainty in momentum is infinite (HINT: you need to Fourier transform ψ). Comment on the relation of this result to the uncertainty principle.

3.11.11 Free Particle Schrodinger Equation

The time-independent Schrodinger equation for a free particle is given by

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial\vec{x}}\right)^2\psi(\vec{x}) = E\psi(\vec{x})$$

It is customary to write $E = \hbar^2 k^2/2m$ to simplify the equation to

$$\left(\nabla^2 + k^2\right)\psi(\vec{x}) = 0$$

Show that

(a) a plane wave $\psi(\vec{x}) = e^{ikz}$

and

(b) a spherical wave $\psi(\vec{x}) = e^{ikr}/r$ ($r = \sqrt{x^2+y^2+z^2}$)

satisfy the equation. Note that in either case, the wavelength of the solution is given by $\lambda = 2\pi/k$ and the momentum by the de Broglie relation $p = \hbar k$.

3.11.12 Double Pinhole Experiment

The double-slit experiment is often used to demonstrate how different quantum mechanics is from its classical counterpart. To avoid mathematical complications with Bessel functions, we will discuss two pinholes rather than two slits. Consider the setup shown below

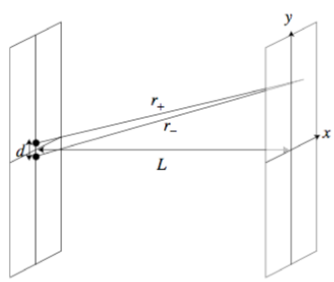

Figure 3.2: The Double Pinhole Setup

Suppose you send in an electron along the $z-$axis onto a screen at $z = 0$ with two pinholes at $x = 0$, $y = \pm d/2$. At a point (x, y) on another screen at $z = L \gg d, \lambda$ the distance from each pinhole is given by $r_\pm = \sqrt{x^2 + (y \mp d/2)^2 + L^2}$.

The spherical waves from each pinhole are added at the point on the screen and hence the wave function is

$$\psi(x, y) = \frac{e^{ikr_+}}{r_+} + \frac{e^{ikr_-}}{r_-}$$

where $k = 2\pi/\lambda$. Answer the following questions.

(a) Considering just the exponential factors, show that constructive interference appears approximately at

$$\frac{y}{r} = n\frac{\lambda}{d} \qquad (n \in \mathbb{Z}) \tag{3.1}$$

where $r = \sqrt{c^2 + y^2 + L^2}$.

(b) Make a plot of the intensity $|\psi(0, y)|^2$ as a function of y, by choosing $k = 1$, $d = 20$ and $L = 1000$, Use the Mathematica Plot function. The intensity $|\psi(0, y)|^2$ is interpreted as the probability distribution for the electron to be detected on the screen, after repeating the same experiment many, many times.

(c) Make a contour plot of the intensity $|\psi(x, y)|^2$ as a function of x and y, for the same parameters, using the Mathematica ContourPlot function.

(d) If you place a counter at both pinholes to see if the electron has passed one of them, all of a sudden the wave function *collapses*. If the electron is observed to pass through the pinhole at $y = +d/2$, the wave function becomes

$$\psi_+(x, y) = \frac{e^{ikr_+}}{r_+}$$

If it is oberved to pass through the pinhole at $y = -d/2$, the wave function becomes

$$\psi_-(x, y) = \frac{e^{ikr_-}}{r_-}$$

After repeating this experiment many times with a 50:50 probability for each of the pinholes, the probability on the screen will be given by

$$|\psi_+(x, y)|^2 + |\psi_-(x, y)|^2$$

instead. Plot this function on the $y-$axis and also show the contour plot to compare its pattern to the case when you do not place a counter. What is the difference from the case without the counter?

Chapter 4

The Mathematics of Quantum Physics:

Dirac Language

4.22 Problems

4.22.1 Simple Basis Vectors

Given two vectors

$$\vec{A} = 7\hat{e}_1 + 6\hat{e}_2 \quad , \quad \vec{B} = -2\hat{e}_1 + 16\hat{e}_2$$

written in the $\{\hat{e}_1, \hat{e}_2\}$ basis set and given another basis set

$$\hat{e}_q = \frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \quad , \quad \hat{e}_p = -\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2$$

(a) Show that $\hat{e}_q$ and $\hat{e}_p$ are orthonormal.

(b) Determine the new components of $\vec{A}$, $\vec{B}$ in the $\{\hat{e}_q, \hat{e}_p\}$ basis set.

4.22.2 Eigenvalues and Eigenvectors

Find the eigenvalues and normalized eigenvectors of the matrix

$$A = \begin{pmatrix} 1 & 2 & 4 \\ 2 & 3 & 0 \\ 5 & 0 & 3 \end{pmatrix}$$

Are the eigenvectors orthogonal? Comment on this.

4.22.3 Orthogonal Basis Vectors

Determine the eigenvalues and eigenstates of the following matrix

$$A = \begin{pmatrix} 2 & 2 & 0 \\ 1 & 2 & 1 \\ 1 & 2 & 1 \end{pmatrix}$$

Using Gram-Schmidt, construct an orthonormal basis set from the eigenvectors of this operator.

4.22.4 Operator Matrix Representation

If the states $\{|1\rangle, |2\rangle\,|3\rangle\}$ form an orthonormal basis and if the operator $\hat{G}$ has the properties

$$\begin{aligned}\hat{G}\,|1\rangle &= 2\,|1\rangle - 4\,|2\rangle + 7\,|3\rangle\\ \hat{G}\,|2\rangle &= -2\,|1\rangle + 3\,|3\rangle\\ \hat{G}\,|3\rangle &= 11\,|1\rangle + 2\,|2\rangle - 6\,|3\rangle\end{aligned}$$

What is the matrix representation of $\hat{G}$ in the $|1\rangle, |2\rangle\,|3\rangle$ basis?

4.22.5 Matrix Representation and Expectation Value

If the states $\{|1\rangle, |2\rangle\,|3\rangle\}$ form an orthonormal basis and if the operator $\hat{K}$ has the properties

$$\begin{aligned}\hat{K}\,|1\rangle &= 2\,|1\rangle\\ \hat{K}\,|2\rangle &= 3\,|2\rangle\\ \hat{K}\,|3\rangle &= -6\,|3\rangle\end{aligned}$$

(a) Write an expression for $\hat{K}$ in terms of its eigenvalues and eigenvectors (projection operators). Use this expression to derive the matrix representing $\hat{K}$ in the $|1\rangle, |2\rangle\,|3\rangle$ basis.

(b) What is the *expectation or average value* of $\hat{K}$, defined as $\langle\alpha|\,\hat{K}\,|\alpha\rangle$, in the state

$$|\alpha\rangle = \frac{1}{\sqrt{83}}\left(-3\,|1\rangle + 5\,|2\rangle + 7\,|3\rangle\right)$$

4.22.6 Projection Operator Representation

Let the states $\{|1\rangle, |2\rangle\,|3\rangle\}$ form an orthonormal basis. We consider the operator given by $\hat{P}_2 = |2\rangle\langle 2|$. What is the matrix representation of this operator? What are its eigenvalues and eigenvectors. For the arbitrary state

$$|A\rangle = \frac{1}{\sqrt{83}}\left(-3\,|1\rangle + 5\,|2\rangle + 7\,|3\rangle\right)$$

What is the result of $\hat{P}_2\,|A\rangle$?

4.22.7 Operator Algebra

An operator for a two-state system is given by

$$\hat{H} = a\left(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\right)$$

where a is a number. Find the eigenvalues and the corresponding eigenkets.

4.22.8 Functions of Operators

Suppose that we have some operator $\hat{Q}$ such that $\hat{Q}\,|q\rangle = q\,|q\rangle$, i.e., $|q\rangle$ is an eigenvector of $\hat{Q}$ with eigenvalue q. Show that $|q\rangle$ is also an eigenvector of the operators $\hat{Q}^2$, $\hat{Q}^n$ and $e^{\hat{Q}}$ and determine the corresponding eigenvalues.

4.22.9 A Symmetric Matrix

Let A be a 4×4 symmetric matrix. Assume that the eigenvalues are given by 0, 1, 2, and 3 with the corresponding normalized eigenvectors

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad , \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} \quad , \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \quad , \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

Find the matrix A.

4.22.10 Determinants and Traces

Let A be an $n \times n$ matrix. Show that

$$\det(\exp(A)) = \exp(Tr(A))$$

4.22.11 Function of a Matrix

Let

$$A = \begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix}$$

Calculate $\exp(\alpha A)$, α real.

4.22.12 More Gram-Schmidt

Let A be the symmetric matrix

$$A = \begin{pmatrix} 5 & -2 & -4 \\ -2 & 2 & 2 \\ -4 & 2 & 5 \end{pmatrix}$$

Determine the eigenvalues and eigenvectors of A. Are the eigenvectors orthogonal to each other? If not, find an orthogonal set using the Gram-Schmidt process.

4.22.13 Infinite Dimensions

Let A be a square finite-dimensional matrix (real elements) such that $AA^T = I$.

(a) Show that $A^T A = I$.

(b) Does this result hold for infinite dimensional matrices?

4.22.14 Spectral Decomposition

Find the eigenvalues and eigenvectors of the matrix

$$M = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Construct the corresponding projection operators, and verify that the matrix can be written in terms of its eigenvalues and eigenvectors. This is the spectral decomposition for this matrix.

4.22.15 Measurement Results

Given particles in state

$$|\alpha\rangle = \frac{1}{\sqrt{83}}\left(-3\,|1\rangle + 5\,|2\rangle + 7\,|3\rangle\right)$$

where $\{|1\rangle, |2\rangle, |3\rangle\}$ form an orthonormal basis, what are the possible experimental results for a measurement of

$$\hat{Y} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix}$$

(written in this basis) and with what probabilities do they occur?

4.22.16 Expectation Values

Let

$$R = \begin{bmatrix} 6 & -2 \\ -2 & 9 \end{bmatrix}$$

represent an observable, and

$$|\Psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

be an arbitrary state vector(with $|a|^2 + |b|^2 = 1$). Calculate $\langle R^2 \rangle$ in two ways:

(a) Evaluate $\langle R^2 \rangle = \langle\Psi|\, R^2\, |\Psi\rangle$ directly.

(b) Find the eigenvalues(r_1 and r_2) and eigenvectors($|r_1\rangle$ and $|r_2\rangle$) of R^2 or R. Expand the state vector as a linear combination of the eigenvectors and evaluate

$$\langle R^2 \rangle = r_1^2\,|c_1|^2 + r_2^2\,|c_2|^2$$

4.22.17 Eigenket Properties

Consider a 3−dimensional ket space. If a certain set of orthonormal kets, say $|1\rangle$, $|2\rangle$ and $|3\rangle$ are used as the basis kets, the operators $\hat{A}$ and $\hat{B}$ are represented by

$$\hat{A} \to \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix} \quad , \quad \hat{B} \to \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}$$

where a and b are both real numbers.

(a) Obviously, $\hat{A}$ has a degenerate spectrum. Does $\hat{B}$ also have a degenerate spectrum?

(b) Show that $\hat{A}$ and $\hat{B}$ commute.

(c) Find a new set of orthonormal kets which are simultaneous eigenkets of both $\hat{A}$ and $\hat{B}$.

4.22.18 The World of Hard/Soft Particles

Let us define a state using a *hardness* basis $\{|h\rangle, |s\rangle\}$, where

$$\hat{O}_{HARDNESS} |h\rangle = |h\rangle \quad , \quad \hat{O}_{HARDNESS} |s\rangle = -|s\rangle$$

and the *hardness* operator $\hat{O}_{HARDNESS}$ is represented by (in this basis) by

$$\hat{O}_{HARDNESS} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Suppose that we are in the state

$$|A\rangle = \cos\theta |h\rangle + e^{i\varphi} \sin\theta |s\rangle$$

(a) Is this state normalized? Show your work. If not, normalize it.

(b) Find the state $|B\rangle$ that is orthogonal to $|A\rangle$. Make sure $|B\rangle$ is normalized.

(c) Express $|h\rangle$ and $|s\rangle$ in the $\{|A\rangle, |B\rangle\}$ basis.

(d) What are the possible outcomes of a hardness measurement on state $|A\rangle$ and with what probability will each occur?

(e) Express the hardness operator in the $\{|A\rangle, |B\rangle\}$ basis.

4.22.19 Things in Hilbert Space

For all parts of this problem, let $\mathcal{H}$ be a Hilbert space spanned by the basis kets $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$, and let a and b be arbitrary complex constants.

(a) Which of the following are Hermitian operators on $\mathcal{H}$?

1. $|0\rangle\langle 1| + i\,|1\rangle\langle 0|$
2. $|0\rangle\langle 0| + |1\rangle\langle 1| + |2\rangle\langle 3| + |3\rangle\langle 2|$
3. $(a\,|0\rangle + |1\rangle)^{+}(a\,|0\rangle + |1\rangle)$
4. $((a\,|0\rangle + b^*\,|1\rangle)^{+}(b\,|0\rangle - a^*\,|1\rangle))\,|2\rangle\langle 1| + |3\rangle\langle 3|$
5. $|0\rangle\langle 0| + i\,|1\rangle\langle 0| - i\,|0\rangle\langle 1| + |1\rangle\langle 1|$

(b) Find the spectral decomposition of the following operator on $\mathcal{H}$:

$$\hat{K} = |0\rangle\langle 0| + 2\,|1\rangle\langle 2| + 2\,|2\rangle\langle 1| - |3\rangle\langle 3|$$

(c) Let $||Psi\rangle$ be a normalized ket in $\mathcal{H}$, and let $\hat{I}$ denote the identity operator on $\mathcal{H}$. Is the operator

$$\hat{B} = \frac{1}{\sqrt{2}}(\hat{I} + |\Psi\rangle\langle\Psi|)$$

a projection operator?

(d) Find the spectral decomposition of the operator $\hat{B}$ from part (c).

4.22.20 A 2-Dimensional Hilbert Space

Consider a 2-dimensional Hilbert space spanned by an orthonormal basis $\{|\uparrow\rangle, |\downarrow\rangle\}$. This corresponds to spin up/down for spin$= 1/2$ as we will see later in Chapter 9. Let us define the operators

$$\hat{S}_x = \frac{\hbar}{2}\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right) \quad , \quad \hat{S}_y = \frac{\hbar}{2i}\left(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|\right) \quad , \quad \hat{S}_z = \frac{\hbar}{2}\left(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|\right)$$

(a) Show that each of these operators is Hermitian.

(b) Find the matrix representations of these operators in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis.

(c) Show that $\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z$, and cyclic permutations. Do this two ways: Using the Dirac notation definitions above and the matrix representations found in (b).

Now let

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \pm |\downarrow\rangle\right)$$

(d) Show that these vectors form a new orthonormal basis.

(e) Find the matrix representations of these operators in the $\{|+\rangle, |-\rangle\}$ basis.

(f) The matrices found in (b) and (e) are related through a *similarity transformation* given by a unitary matrix, U, such that

$$\hat{S}_x^{(\uparrow\downarrow)} = U^\dagger \hat{S}_x^{(\pm)} U \quad , \quad \hat{S}_y^{(\uparrow\downarrow)} = U^\dagger \hat{S}_y^{(\pm)} U \quad , \quad \hat{S}_z^{(\uparrow\downarrow)} = U^\dagger \hat{S}_z^{(\pm)} U$$

where the superscript denotes the basis in which the operator is represented. Find U and show that it is unitary.

Now let

$$\hat{S}_\pm = \frac{1}{2}\left(\hat{S}_x \pm i\hat{S}_y\right)$$

(g) Express $\hat{S}_\pm$ as outer products in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis and show that $\hat{S}_+^\dagger = \hat{S}_-$.

(h) Show that

$$\hat{S}_+ |\downarrow\rangle = |\uparrow\rangle \ , \ \hat{S}_- |\uparrow\rangle = |\downarrow\rangle \ , \ \hat{S}_- |\downarrow\rangle = 0 \ , \ \hat{S}_+ |\uparrow\rangle = 0$$

and find

$$\langle\uparrow| \hat{S}_+ \ , \ \langle\downarrow| \hat{S}_+ \ , \ \langle\uparrow| \hat{S}_- \ , \ \langle\downarrow| \hat{S}_-$$

4.22.21 Find the Eigenvalues

The three matrices M_x, M_y, M_z, each with 256 rows and columns, obey the commutation rules

$$[M_i, M_j] = i\hbar\varepsilon_{ijk}M_k$$

The eigenvalues of M_z are $\pm 2\hbar$ (each once), $\pm 2\hbar$ (each once), $\pm 3\hbar/2$ (each 8 times), $\pm\hbar$ (each 28 times), $\pm\hbar/2$ (each 56 times), and 0 (70 times). State the 256 eigenvalues of the matrix $M^2 = M_x^2 + M_y^2 + M_z^2$.

4.22.22 Operator Properties

(a) If O is a quantum-mechanical operator, what is the definition of the corresponding Hermitian conjugate operator, O^+?

(b) Define what is meant by a Hermitian operator in quantum mechanics.

(c) Show that d/dx is not a Hermitian operator. What is its Hermitian conjugate, $(d/dx)^+$?

(d) Prove that for any two operators A and B, $(AB)^+ = B^+A^+$,

4.22.23 Ehrenfest's Relations

Show that the following relation applies for any operator O that lacks an explicit dependence on time:

$$\frac{\partial}{\partial t}\langle O\rangle = \frac{i}{\hbar}\langle [H, O]\rangle$$

HINT: Remember that the Hamiltonian, H, is a Hermitian operator, and that H appears in the time-dependent Schrodinger equation.

Use this result to derive Ehrenfest's relations, which show that classical mechanics still applies to expectation values:

$$m\frac{\partial}{\partial t}\langle\vec{x}\rangle = \langle\vec{p}\rangle \quad , \quad \frac{\partial}{\partial t}\langle\vec{p}\rangle = -\langle\nabla V\rangle$$

4.22.24 Solution of Coupled Linear ODEs

Consider the set of coupled linear differential equations $\dot{x} = Ax$ where $x = (x_1, x_2, x_3) \in R^3$ and

$$A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

(a) Find the general solution $x(t)$ in terms of $x(0)$ by matrix exponentiation.

(b) Using the results from part (a), write the general solution $x(t)$ by expanding $x(0)$ in eigenvectors of A. That is, write

$$x(t) = e^{\lambda_1} c_1 v_1 + e^{\lambda_2} c_2 v_2 + e^{\lambda_3} c_3 v_3$$

where (λ_i, v_i) are the eigenvalue-eigenvector pairs for A and the c_i are coefficients written in terms of the $x(0)$.

4.22.25 Spectral Decomposition Practice

Find the spectral decomposition of the matrix

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{pmatrix}$$

4.22.26 More on Projection Operators

The basic definition of a projection operator is that it must satisfy $P^2 = P$. If P furthermore satisfies $P = P^+$ we say that P is an orthogonal projector. As we derived in the text, the eigenvalues of an orthogonal projector are all equal to either zero or one.

(a) Show that if P is a projection operator, then so is $I - P$.

(b) Show that for any orthogonal projector P and an normalized state, $0 \leq \langle P \rangle \leq 1$.

(c) Show that the singular values of an orthogonal projector are also equal to zero or one. The singular values of an arbitrary matrix A are given by the square-roots of the eigenvalues of A^+A. It follows that for every singular value σ_i of a matrix A there exist some unit normalized vector u_i such that

$$u_i^+ A^+ A u_i = \sigma_i^2$$

Conclude that the action of an orthogonal projection operator never lengthens a vector (never increases its norm).

For the next two parts we consider the example of a non-orthogonal projection operator

$$N = \begin{pmatrix} 0 & 0 \\ -1 & 1 \end{pmatrix}$$

(d) Find the eigenvalues and eigenvectors of N. Does the usual spectral decomposition work as a representation of N?

(e) Find the singular values of N. Can you interpret this in terms of the action of N on vectors in R^2?

Chapter 5

Probability

5.6 Problems

5.6.1 Simple Probability Concepts

There are 14 short problems in this section. If you have not studied any probability ideas before using this book, then these are all new to you and doing them should enable you to learn the basic ideas of probability methods. If you have studied probability ideas before, these should all be straightforward.

(a) Two dice are rolled, one after the other. Let A be the event that the second number if greater than the first. Find $P(A)$.

(b) Three dice are rolled and their scores added. Are you more likely to get 9 than 10, or vice versa?

(c) Which of these two events is more likely?

1. four rolls of a die yield at least one six
2. twenty-four rolls of two dice yield at least one double six

(d) From meteorological records it is known that for a certain island at its winter solstice, it is wet with probability 30%, windy with probability 40% and both wet and windy with probability 20%. Find

(1) $Prob$(dry)
(2) $Prob$(dry AND windy)
(3) $Prob$(wet OR windy)

(e) A kitchen contains two fire alarms; one is activated by smoke and the other by heat. Experiment has shown that the probability of the smoke alarm sounding within one minute of a fire starting is 0.95, the probability of the heat alarm sounding within one minute of a fire starting is 0.91, and the probability of both alarms sounding within one minute is 0.88. What is the probability of at least one alarm sounding within a minute?

(f) Suppose you are about to roll two dice, one from each hand. What is the probability that your right-hand die shows a larger number than your left-hand die? Now suppose you roll the left-hand die first and it shows 5. What is the probability that the right-hand die shows a larger number?

(g) A coin is flipped three times. Let A be the event that the first flip gives a head and B be the event that there are exactly two heads overall. Determine

(1) $P(A|B)$

(2) $P(B|A)$

(h) A box contains a double-headed coin, a double-tailed coin and a conventional coin. A coin is picked at random and flipped. It shows a head. What is the probability that it is the double-headed coin?

(i) A box contains 5 red socks and 3 blue socks. If you remove 2 socks at random, what is the probability that you are holding a blue pair?

(j) An inexpensive electronic toy made by Acme Gadgets Inc. is defective with probability 0.001. These toys are so popular that they are copied and sold illegally but cheaply. Pirate versions capture 10% of the market and any pirated copy is defective with probability 0.5. If you buy a toy, what is the chance that it is defective?

(k) Patients may be treated with any one of a number of drugs, each of which may give rise to side effects. A certain drug C has a 99% success rate in the absence of side effects and side effects only arise in 5% of cases. However, if they do arise, then C only has a 30% success rate. If C is used, what is the probability of the event A that a cure is effected?

(l) Suppose a multiple choice question has c available choices. A student either knows the answer with probability p or guesses at random with probability $1 - p$. Given that the answer selected is correct, what is the probability that the student knew the answer?

(m) Common PINs do not begin with zero. They have four digits. A computer assigns you a PIN at random. What is the probability that all four digits are different?

(n) You are dealt a hand of 5 cards from a conventional deck(52 cards). A full house comprises 3 cards of one value and 2 of another value. If that hand has 4 cards of one value, this is called four of a kind. Which is more likely?

5.6.2 Playing Cards

Two cards are drawn at random from a shuffled deck and laid aside without being examined. Then a third card is drawn. Show that the probability that the third card is a spade is 1/4 just as it was for the first card. *HINT*: Consider all the (mutually exclusive) possibilities (two discarded cards spades, third card spade or not spade, etc).

5.6.3 Birthdays

What is the probability that you and a friend have different birthdays? (for simplicity let a year have 365 days). What is the probability that three people have different birthdays? Show that the probability that n people have different birthdays is

$$p = \left(1 - \frac{1}{365}\right)\left(1 - \frac{2}{365}\right)\left(1 - \frac{3}{365}\right) \ldots.. \left(1 - \frac{n-1}{365}\right)$$

Estimate this for $n << 365$ by calculating $\log(p)$ (use the fact that $\log(1+x) \approx x$ for $x \ll 1$). Find the smallest integer N for which $p < 1/2$. Hence show that for a group of N people or more, the probability is greater than 1/2 that two of them have the same birthday.

5.6.4 Is there life?

The number of stars in our galaxy is about $N = 10^{11}$. Assume that the probability that a star has planets is $p = 10^{-2}$, the probability that the conditions on the planet are suitable for life is $q = 10^{-2}$, and the probability of life evolving, given suitable conditions, is $r = 10^{-2}$. These numbers are rather arbitrary.

(a) What is the probability of life existing in an arbitrary solar system (a star and planets, if any)?

(b) What is the probability that life exists in at least one solar system?

5.6.5 Law of large Numbers

This problem illustrates the law of large numbers.

(a) Assuming the probability of obtaining *heads* in a coin toss is 0.5, compare the probability of obtaining *heads* in 5 out of 10 tosses with the probability of obtaining *heads* in 50 out of 100 tosses and with the probability of obtaining *heads* in 5000 out of 10000 tosses. What is happening?

(b) For a set of 10 tosses, a set of 100 tosses and a set of $10000 tosses$, calculate the probability that the fraction of *heads* will be between 0.445 and 0.555. What is happening?

5.6.6 Bayes

Suppose that you have 3 nickels and 4 dimes in your right pocket and 2 nickels and a quarter in your left pocket. You pick a pocket at random and from it select a coin at random. If it is a nickel, what is the probability that it came from your right pocket? Use Baye's formula.

5.6.7 Psychological Tests

Two psychologists reported on tests in which subjects were given the *prior information*:

> I = In a certain city, 85% of the taxicabs
> are blue and 15% are green

and the *data*:

> D = A witness to a crash who is 80% reliable (i.e.,
> who in the lighting conditions prevailing can
> distinguish between green and blue 80% of the
> time) reports that the taxicab involved in the
> crash was green

The subjects were then asked to judge the probability that the taxicab was actually blue. What is the correct answer?

5.6.8 Bayes Rules, Gaussians and Learning

Let us consider a classical problem(no quantum uncertainty). Suppose we are trying to measure the position of a particle and we assign a prior probability function,

$$p(x) = \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-(x-x_0)^2/2\sigma_0^2}$$

Our measuring device is not perfect. Due to noise it can only measure with a resolution Δ, i.e., when I measure the position, I must assume error bars of this size. Thus, if my detector registers the position as y, I assign the likelihood that the position was x by a Gaussian,

$$p(y|x) = \frac{1}{\sqrt{2\pi\Delta^2}} e^{-(y-x)^2/2\Delta^2}$$

Use Bayes theorem to show that, given the new data, I must now update my probability assignment of the position to a new Gaussian,

$$p(x|y) = \frac{1}{\sqrt{2\pi\sigma'^2}} e^{-(x-x')^2/2\sigma'^2}$$

where

$$x' = x_0 + K_1(y - x_0) \ , \ \sigma'^2 = K_2\sigma_0^2 \ , \ K_1 = \frac{\sigma_0^2}{\sigma_0^2 + \Delta^2} \ , \ K_2 = \frac{\Delta^2}{\sigma_0^2 + \Delta^2}$$

Comment on the behavior as the measurement resolution improves. How does the learning process work?

5.6.9 Berger's Burgers-Maximum Entropy Ideas

A fast food restaurant offers three meals: burger, chicken, and fish. The price, Calorie count, and probability of each meal being delivered cold are listed below in Table 5.1:

Item	Entree	Cost	Calories	Prob(hot)	Prob(cold)
Meal 1	burger	\$1.00	1000	0.5	0.5
Meal 2	chicken	\$2.00	600	0.8	0.2
Meal 3	fish	\$3.00	400	0.9	0.1

Table 5.1: Berger's Burgers Details

We want to identify the state of the system, i.e., the values of

$$\begin{aligned} Prob(burger) &= P(B) \\ Prob(chicken) &= P(C) \\ Prob(fish) &= P(F) \end{aligned}$$

Even though the problem has now been set up, we do not know which state the actual state of the system. To express what we do know despite this ignorance, or uncertainty, we assume that each of the possible states A_i has some probability of occupancy $P(A_i)$, where i is an index running over the possible states. As stated above, for the restaurant model, we have three such possibilities, which we have labeled $P(B)$, $P(C)$, and $P(F)$.

A probability distribution $P(A_i)$ has the property that each of the probabilities is in the range $0 \leq P(A_i) \leq 1$ and since the events are mutually exclusive and exhaustive, the sum of all the probabilities is given by

$$1 = \sum_i P(A_i) \tag{5.1}$$

Since probabilities are used to cope with our lack of knowledge and since one person may have more knowledge than another, it follows that two observers may, because of their different knowledge, use different probability distributions. In this sense probability, and all quantities that are based on probabilities are *subjective*.

Our uncertainty is expressed quantitatively by the *information* which we do not have about the state occupied. This *information* is

$$S = \sum_i P(A_i) \log_2 \left(\frac{1}{P(A_i)} \right) \tag{5.2}$$

This *information* is measured in bits because we are using logarithms to base 2.

In physical systems, this uncertainty is known as the *entropy*. Note that the entropy, because it is expressed in terms of probabilities, depends on the observer.

The principle of maximum entropy (**MaxEnt**) is used to discover the probability distribution which leads to the largest value of the entropy (a maximum), thereby assuring that no information is inadvertently assumed.

If one of the probabilities is equal to 1, the all the other probabilities are equal to 0, and the entropy is equal to 0.

It is a property of the above entropy formula that it has its maximum when all the probabilities are equal (for a finite number of states), which the state of *maximum ignorance*.

If we have no additional information about the system, then such a result seems reasonable. However, if we have additional information, then we should be able to find a probability distribution which is better in the sense that it has less uncertainty.

In this problem we will impose only one constraint. The particular constraint is the known average price for a meal at Berger's Burgers, namely $1.75. This constraint is an example of an expected value.

(a) Express the constraint in terms of the unknown probabilities and the prices for the three types of meals.

(b) Using this constraint and the total probability equal to 1 rule find possible ranges for the three probabilities in the form

$$\begin{aligned} a &\leq P(B) \leq b \\ c &\leq P(C) \leq d \\ e &\leq P(F) \leq f \end{aligned}$$

(c) Using this constraint, the total probability equal to 1 rule, the entropy formula and the MaxEnt rule, find the values of $P(B)$, $P(C)$, and $P(F)$ which maximize S.

(d) For this state determine the expected value of Calories and the expected number of meals served cold.

In finding the state which maximizes the entropy, we found the probability distribution that is consistent with the constraints and has the largest uncertainty. Thus, we have not inadvertently introduced any biases into the probability estimation.

5.6.10 Extended Menu at Berger's Burgers

Suppose now that Berger's extends its menu to include a Tofu option as shown in Table 5.2 below:

Entree	Cost	Calories	Prob(hot)	Prob(cold)
burger	\$1.00	1000	0.5	0.5
chicken	\$2.00	600	0.8	0.2
fish	\$3.00	400	0.9	0.1
tofu	\$8.00	200	0.6	0.4

Table 5.2: Extended Berger's Burgers Menu Details

Suppose you are now told that the average meal price is \$2.50.

Use the method of Lagrange multipliers to determine the state of the system (i.e., $P(B)$, $P(C)$, $P(F)$ and $P(T)$).

You will need to solve some equations numerically.

5.6.11 The Poisson Probability Distribution

The arrival time of rain drops on the roof or photons from a laser beam on a detector are completely random, with no correlation from count to count. If we count for a certain time interval we won't always get the same number - it will fluctuate from shot-to-shot. This kind of noise is sometimes known as *shot noise* or *counting statistics*.

Suppose the particles arrive at an average rate R. In a small time interval $\Delta t \ll 1/R$ no more than one particle can arrive. We seek the probability for n particles to arrive after a time t, $P(n,t)$.

(a) Show that the probability to detect zero particles exponentially decays, $P(0,t) = e^{-Rt}$.

(b) Obtain a differential equation as a recursion relation

$$\frac{d}{dt}P(n,t) + RP(n,t) = RP(n-1,t)$$

(c) Solve this to find the Poisson distribution

$$P(n,t) = \frac{(Rt)^n}{n!}e^{-Rt}$$

Plot a histogram for $Rt = 0.1, 1.0, 10.0$.

(d) Show that the mean and standard deviation in number of counts are:

$$\langle n \rangle = Rt \quad , \quad \sigma_n = \sqrt{Rt} = \sqrt{\langle n \rangle}$$

[HINT: To find the variance consider $\langle n(n-1) \rangle$].

Fluctuations going as the square root of the mean are characteristic of counting statistics.

(e) An alternative way to derive the Poisson distribution is to note that the count in each small time interval is a Bernoulli trial(find out what this is), with probability $p = R\Delta t$ to detect a particle and $1 - p$ for no detection. The total number of counts is thus the binomial distribution. We need to take the limit as $\Delta t \to 0$ (thus $p \to 0$) but Rt remains finite (this is just calculus). To do this let the total number of intervals $N = t/\Delta t \to \infty$ while $Np = Rt$ remains finite. Take this limit to get the Poisson distribution.

5.6.12 Modeling Dice: Observables and Expectation Values

Suppose we have a pair of six-sided dice. If we roll them, we get a pair of results

$$a \in \{1, 2, 3, 4, 5, 6\} \quad , \quad b \in \{1, 2, 3, 4, 5, 6\}$$

where a is an observable corresponding to the number of spots on the top face of the first die and b is an observable corresponding to the number of spots on the top face of the second die. If the dice are fair, then the probabilities for the roll are

$$Pr(a = 1) = Pr(a = 2) = Pr(a = 3) = Pr(a = 4) = Pr(a = 5) = Pr(a = 6) = 1/6$$
$$Pr(b = 1) = Pr(b = 2) = Pr(b = 3) = Pr(b = 4) = Pr(b = 5) = Pr(b = 6) = 1/6$$

Thus, the expectation values of a and b are

$$\langle a \rangle = \sum_{i=1}^{6} i Pr(a = i) = \frac{1 + 2 + 3 + 4 + 5 + 6}{6} = 7/2$$
$$\langle b \rangle = \sum_{i=1}^{6} i Pr(b = i) = \frac{1 + 2 + 3 + 4 + 5 + 6}{6} = 7/2$$

Let us define two new observables in terms of a and b:

$$s = a + b \quad , \quad p = ab$$

Note that the possible values of s range from 2 to 12 and the possible values of p range from 1 to 36. Perform an explicit computation of the expectation values of s and p by writing out

$$\langle s\rangle = \sum_{i=2}^{12} iPr(s=i)$$

and

$$\langle p\rangle = \sum_{i=1}^{36} iPr(p=i)$$

Do this by explicitly computing all the probabilities $Pr(s=i)$ and $Pr(p=i)$. You should find that $\langle s\rangle = \langle a\rangle + \langle b\rangle$ and $\langle p\rangle = \langle a\rangle\langle b\rangle$. Why are these results not surprising?

5.6.13 Conditional Probabilities for Dice

Use the results of Problem 5.12. You should be able to intuit the correct answers for this problems by straightforward probabilistic reasoning; if not you can use Baye's Rule

$$Pr(x|y) = \frac{Pr(y|x)Pr(x)}{Pr(y)}$$

to calculate the results. Here $Pr(x|y)$ represents *the probability of x given y*, where x and y should be propositions of equations (for example, $Pr(a=2|s=8)$ is the probability that $a=2$ given the $s=8$).

(a) Suppose your friend rolls a pair of dice and, without showing you the result, tells you that $s=8$. What is your conditional probability distribution for a?

(b) Suppose your friend rolls a pair of dice and, without showing you the result, tells you that $p=12$. What is your conditional expectation value for s?

5.6.14 Matrix Observables for Classical Probability

Suppose we have a biased coin, which has probability p_h of landing heads-up and probability p_t of landing tails-up. Say we flip the biased coin but do not look at the result. Just for fun, let us represent this preparation procedure by a *classical state vector*

$$x_0 = \begin{pmatrix} \sqrt{p_h} \\ \sqrt{p_t} \end{pmatrix}$$

(a) Define an observable (random variable) r that takes value $+1$ if the coin is heads-up and -1 if the coin is tails-up. Find a matrix R such that

$$x_0^T R x_0 = \langle r\rangle$$

where $\langle r\rangle$ denotes the mean, or expectation value, of our observable.

(b) Now find a matrix F such that the *dynamics* corresponding to turning the coin over (after having flipped it, but still without looking at the result) is represented by

$$x_0 \mapsto F x_0$$

and

$$\langle r \rangle \mapsto x_0^T F^T R F x_0$$

Does $U = F^T R F$ make sense as an observable? If so explain what values it takes for a coin-flip result of heads or tails. What about RF or $F^T R$?

(c) Let us now define the algebra of flipped-coin observables to be the set V of all matrices of the form

$$v = aR + bR^2 \quad , \quad a, b \in R$$

Show that this set is closed under matrix multiplication and that it is commutative. In other words, for any $v_1, v_2 \in V$, show that

$$v_1, v_2 \in V \quad , \quad v_1 v_2 = v_2 v_1$$

Is U in this set? How should we interpret the observable represented by an arbitrary element $v \in V$?

Chapter 6

The Formulation of Quantum Mechanics

6.19 Problems

6.19.1 Can It Be Written?

Show that a density matrix $\hat{\rho}$ represents a state vector (i.e., it can be written as $|\psi\rangle\langle\psi|$ for some vector $|\psi\rangle$) if, and only if,

$$\hat{\rho}^2 = \hat{\rho}$$

6.19.2 Pure and Nonpure States

Consider an observable σ that can only take on two values $+1$ or -1. The eigenvectors of the corresponding operator are denoted by $|+\rangle$ and $|-\rangle$. Now consider the following states.

(a) The one-parameter family of pure states that are represented by the vectors

$$|\theta\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{e^{i\theta}}{\sqrt{2}}|-\rangle$$

for arbitrary θ.

(b) The nonpure state

$$\rho = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-|$$

Show that $\langle\sigma\rangle = 0$ for both of these states. What, if any, are the physical differences between these various states, and how could they be measured?

6.19.3 Probabilities

Suppose the operator

$$M = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

represents an observable. Calculate the probability $Prob(M = 0|\rho)$ for the following state operators:

$$(a)\ \ \rho = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \quad , \quad (b)\ \ \rho = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \quad , \quad (c)\ \ \rho = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} \end{bmatrix}$$

6.19.4 Acceptable Density Operators

Which of the following are acceptable as state operators? Find the corresponding state vectors for any of them that represent pure states.

$$\rho_1 = \begin{bmatrix} \frac{1}{4} & \frac{3}{4} \\ \frac{3}{4} & \frac{3}{4} \end{bmatrix} \quad , \quad \rho_2 = \begin{bmatrix} \frac{9}{25} & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{25} \end{bmatrix}$$

$$\rho_3 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & \frac{1}{2} & 0 \\ \frac{1}{4} & 0 & 0 \end{bmatrix} \quad , \quad \rho_4 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} \end{bmatrix}$$

$$\rho_5 = \frac{1}{3}\left|u\right\rangle\left\langle u\right| + \frac{2}{3}\left|v\right\rangle\left\langle v\right| + \frac{\sqrt{2}}{3}\left|u\right\rangle\left\langle v\right| + \frac{\sqrt{2}}{3}\left|v\right\rangle\left\langle u\right|$$
$$\langle u \mid u\rangle = \langle v \mid v\rangle = 1 \text{and}\ \langle u \mid v\rangle = 0$$

6.19.5 Is it a Density Matrix?

Let $\hat{\rho}_1$ and $\hat{\rho}_2$ be a pair of density matrices. Show that

$$\hat{\rho} = r\hat{\rho}_1 + (1-r)\hat{\rho}_2$$

is a density matrix for all real numbers r such that $0 \leq r \leq 1$.

6.19.6 Unitary Operators

An important class of operators are unitary, defined as those that preserve inner products, i.e., if $\left|\tilde{\psi}\right\rangle = \hat{U}\left|\psi\right\rangle$ and $\left|\tilde{\varphi}\right\rangle = \hat{U}\left|\varphi\right\rangle$, then $\left\langle \tilde{\varphi} \,\middle|\, \tilde{\psi}\right\rangle = \langle \varphi \mid \psi\rangle$ and $\left\langle \tilde{\psi} \,\middle|\, \tilde{\varphi}\right\rangle = \langle \psi \mid \varphi\rangle$.

(a) Show that unitary operators satisfy $\hat{U}\hat{U}^+ = \hat{U}^+\hat{U} = \hat{I}$, i.e., the adjoint is the inverse.

(b) Consider $\hat{U} = e^{i\hat{A}}$, where $\hat{A}$ is a Hermitian operator. Show that $\hat{U}^+ = e^{-i\hat{A}}$ and thus show that $\hat{U}$ is unitary.

(c) Let $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ where t is time and $\hat{H}$ is the Hamiltonian. Let $\left|\psi(0)\right\rangle$ be the state at time $t = 0$. Show that $\left|\psi(t)\right\rangle = \hat{U}(t)\left|\psi(0)\right\rangle = e^{-i\hat{H}t/\hbar}\left|\psi(0)\right\rangle$ is a solution of the time-dependent Schrodinger equation, i.e., the state evolves according to a unitary map. Explain why this is required by the conservation of probability in non-relativistic quantum mechanics.

(d) Let $\{|u_n\rangle\}$ be a complete set of energy eigenfunctions, $\hat{H}|u_n\rangle = E_n|u_n\rangle$. Show that $\hat{U}(t) = \sum_n e^{-iE_n t/\hbar}|u_n\rangle\langle u_n|$. Using this result, show that $|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar}|u_n\rangle$. What is c_n?

6.19.7 More Density Matrices

Suppose we have a system with total angular momentum 1. Pick a basis corresponding to the three eigenvectors of the $z-$component of the angular momentum, J_z, with eigenvalues $+1$, 0, -1, respectively. We are given an ensemble of such systems described by the density matrix

$$\rho = \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

(a) Is ρ a permissible density matrix? Give your reasoning. For the remainder of this problem, assume that it is permissible. Does it describe a pure or mixed state? Give your reasoning.

(b) Given the ensemble described by ρ, what is the average value of J_z?

(c) What is the spread (standard deviation) in the measured values of J_z?

6.19.8 Scale Transformation

Space is invariant under the scale transformation

$$x \to x' = e^c x$$

where c is a parameter. The corresponding unitary operator may be written as

$$\hat{U} = e^{-ic\hat{D}}$$

where $\hat{D}$ is the *dilation* generator. Determine the commutators $\left[\hat{D}, \hat{x}\right]$ and $\left[\hat{D}, \hat{p}_x\right]$ between the generators of dilation and space displacements. Determine the operator $\hat{D}$. Not all the laws of physics are invariant under dilation, so the symmetry is less common than displacements or rotations. You will need to use the identity in Problem 6.11.

6.19.9 Operator Properties

(a) Prove that if $\hat{H}$ is a Hermitian operator, then $U = e^{iH}$ is a unitary operator.

(b) Show that $\det U = e^{iTrH}$.

6.19.10 An Instantaneous Boost

The unitary operator

$$\hat{U}(\vec{v}) = e^{i\vec{v}\cdot\hat{G}}$$

describes the instantaneous ($t = 0$) effect of a transformation to a frame of reference moving at the velocity $\vec{v}$ with respect to the original reference frame. Its effects on the velocity and position operators are:

$$\hat{U}\hat{V}\hat{U}^{-1} = \hat{V} - \vec{v}\hat{I} \quad , \quad \hat{U}\hat{Q}\hat{U}^{-1} = \hat{Q}$$

Find an operator $\hat{G}_t$ such that the unitary operator $\hat{U}(\vec{v},t) = e^{i\vec{v}\cdot\hat{G}_t}$ will yield the full Galilean transformation

$$\hat{U}\hat{V}\hat{U}^{-1} = \hat{V} - \vec{v}\hat{I} \quad , \quad \hat{U}\hat{Q}\hat{U}^{-1} = \hat{Q} - \vec{v}t\hat{I}$$

Verify that $\hat{G}_t$ satisfies the same commutation relation with $\vec{P}$, $\vec{J}$ and $\hat{H}$ as does $\hat{G}$.

6.19.11 A Very Useful Identity

Prove the following identity, in which $\hat{A}$ and $\hat{B}$ are operators and x is a parameter.

$$e^{x\hat{A}}\hat{B}e^{-x\hat{A}} = \hat{B} + \left[\hat{A},\hat{B}\right]x + \left[\hat{A},\left[\hat{A},\hat{B}\right]\right]\frac{x^2}{2} + \left[\hat{A},\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]\right]\frac{x^3}{6} + ...$$

There is a clever way(see Problem 6.12 below if you are having difficulty) to do this problem using ODEs and not just brute-force multiplying everything out.

6.19.12 A Very Useful Identity with some help....

The operator $U(a) = e^{ipa/\hbar}$ is a translation operator in space (here we consider only one dimension). To see this we need to prove the identity

$$\begin{aligned} e^{A}Be^{-A} &= \sum_{0}^{\infty}\frac{1}{n!}\underbrace{[A,[A,...[A,}_{n}B\underbrace{]....]]}_{n} \\ &= B + [A,B] + \frac{1}{2!}[A,[A,B]] + \frac{1}{3!}[A,[A,[A,B]]] + ... \end{aligned}$$

(a) Consider $B(t) = e^{tA}Be^{-tA}$, where t is a real parameter. Show that

$$\frac{d}{dt}B(t) = e^{tA}[A,B]e^{-tA}$$

(b) Obviously, $B(0) = B$ and therefore

$$B(1) = B + \int_0^1 dt\,\frac{d}{dt}B(t)$$

Now using the power series $B(t) = \sum_{n=0}^{\infty} t^n B_n$ and using the above integral expressio, show that $B_n = [A, B_{n-1}]/n$.

(c) Show by induction that

$$B_n = \frac{1}{n!}\underbrace{[A,[A,...[A,}_{n}B\underbrace{]....]]}_{n}$$

(d) Use $B(1) = e^A B e^{-A}$ and prove the identity.

(e) Now prove $e^{ipa/\hbar} x e^{-ipa/\hbar} = x + a$ showing that $U(a)$ indeed translates space.

6.19.13 Another Very Useful Identity

Prove that

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}[\hat{A},\hat{B}]}$$

provided that the operators $\hat{A}$ and $\hat{B}$ satisfy

$$\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] = \left[\hat{B},\left[\hat{A},\hat{B}\right]\right] = 0$$

A clever solution uses Problem 6.11or 6.12 result and ODEs.

6.19.14 Pure to Nonpure?

Use the equation of motion for the density operator $\hat{\rho}$ to show that a pure state cannot evolve into a nonpure state and vice versa.

6.19.15 Schur's Lemma

Let G be the space of complex differentiable test functions, $g(x)$, where x is real. It is convenient to extend G slightly to encompass all functions, $\tilde{g}(x)$, such that $\tilde{g}(x) = g(x) + c$, where $g \in G$ and c is any constant. Let us call the extended space $\tilde{G}$. Let $\hat{q}$ and $\hat{p}$ be linear operators on $\tilde{G}$ such that

$$\begin{aligned} \hat{q}g(x) &= xg(x) \\ \hat{p}g(x) &= -i\frac{dg(x)}{dx} = -ig'(x) \end{aligned}$$

Suppose $\hat{M}$ is a linear operator on $\tilde{G}$ that commutes with $\hat{q}$ and $\hat{p}$. Show that

(1) $\hat{q}$ and $\hat{p}$ are hermitian on $\tilde{G}$

(2) $\hat{M}$ is a constant multiple of the identity operator

6.19.16 More About the Density Operator

Let us try to improve our understanding of the density matrix formalism and the connections with *information* or *entropy.*We consider a simple two-state system. Let ρ be any general density matrix operating on the two-dimensional Hilbert space of this system.

(a) Calculate the entropy, $s = -Tr(\rho \ln \rho)$ corresponding to this density matrix. Express the result in terms of a single real parameter. Make a clear interpretation of this parameter and specify its range.

(b) Make a graph of the entropy as a function of the parameter. What is the entropy for a pure state? Interpret your graph in terms of knowledge about a system taken from an ensemble with density matrix ρ.

(c) Consider a system with ensemble ρ a mixture of two ensembles ρ_1 and ρ_2:

$$\rho = \theta\rho_1 + (1-\theta)\rho_2 \quad , \quad 0 \leq \theta \leq 1$$

As an example, suppose

$$\rho_1 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad \rho_2 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

in some basis. Prove that

$$s(\rho) \geq \rho = \theta s(\rho_1) + (1-\theta)s(\rho_2)$$

with equality if $\theta = 0$ or $\theta = 1$. This the so-called *von Neumann's mixing theorem.*

6.19.17 Entanglement and the Purity of a Reduced Density Operator

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ and $\{|0_B\rangle, |1_B\rangle\}$. Let $|\Psi_{AB}\rangle$ be the state

$$|\Psi_{AB}\rangle = \cos\theta\,|0_A\rangle \otimes |0_B\rangle + \sin\theta\,|1_A\rangle \otimes |1_B\rangle$$

For $0 < \theta < \pi/2$, this is an entangled state. The purity ζ of the reduced density operator $\tilde{\rho}_A = Tr_B[|\Psi_{AB}\rangle\langle\Psi_{AB}|]$ given by

$$\zeta = Tr[\tilde{\rho}_A^2]$$

is a good measure of the *entanglement* of states in $\mathcal{H}_{AB}$. For pure states of the above form, find extrema of ζ with respect to θ ($0 \leq \theta \leq \pi/2$). Do entangled states have large ζ or small ζ?

6.19.18 The Controlled-Not Operator

Again let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ and $\{|0_B\rangle, |1_B\rangle\}$. Consider the *controlled-not* operator on $\mathcal{H}_{AB}$ (very important in quantum computing),

$$U_{AB} = P_0^A \otimes I^B + P_1^A \otimes \sigma_x^B$$

where $P_0^A = |0_A\rangle \langle 0_A|$, $P_1^A = |1_A\rangle \langle 1_A|$ and $\sigma_x^B = |0_B\rangle \langle 1_B| + |1_B\rangle \langle 0_0|$.

Write a matrix representation for U_{AB} with respect to the following (ordered) basis for $\mathcal{H}_{AB}$

$$|0_A\rangle \otimes |0_B\rangle \ , \ |0_A\rangle \otimes |1_B\rangle \ , \ |1_A\rangle \otimes |0_B\rangle \ , \ |1_A\rangle \otimes |1_B\rangle$$

Find the eigenvectors of U_{AB} - you should be able to do this by inspection. Do any of them correspond to entangled states?

6.19.19 Creating Entanglement via Unitary Evolution

Working with the same system as in Problems 6.17 and 6.18, find a factorizable *input* state

$$\left|\Psi_{AB}^{in}\right\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$$

such that the *output* state

$$\left|\Psi_{AB}^{out}\right\rangle = U_{AB} \left|\Psi_{AB}^{in}\right\rangle$$

is *maximally entangled*. That is, find any factorizable $\left|\Psi_{AB}^{in}\right\rangle$ such that $Tr[\tilde{\rho}_A^2] = 1/2$, where

$$\tilde{\rho}_A = Tr_B[\left|\Psi_{AB}^{out}\right\rangle \left\langle\Psi_{AB}^{out}\right|]$$

6.19.20 Tensor-Product Bases

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ and $\{|0_B\rangle, |1_B\rangle\}$. Consider the following entangled state in the joint Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$,

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} \left(|0_A 1_B\rangle + |1_A 0_B\rangle\right)$$

where $|0_A 1_B\rangle$ is short-hand notation for $|0_A\rangle \otimes |1_B\rangle$ and so on. Rewrite this state in terms of a new basis $\{\left|\tilde{0}_A\tilde{0}_B\right\rangle, \left|\tilde{0}_A\tilde{1}_B\right\rangle, \left|\tilde{1}_A\tilde{0}_B\right\rangle, \left|\tilde{1}_A\tilde{1}_B\right\rangle\}$, where

$$\left|\tilde{0}_A\right\rangle = \cos\frac{\phi}{2}|0_A\rangle + \sin\frac{\phi}{2}|1_A\rangle$$
$$\left|\tilde{1}_A\right\rangle = -\sin\frac{\phi}{2}|0_A\rangle + \cos\frac{\phi}{2}|1_A\rangle$$

and similarly for $\{\left|\tilde{0}_B\right\rangle, \left|\tilde{1}_B\right\rangle\}$. Again $\left|\tilde{0}_A\tilde{0}_B\right\rangle = \left|\tilde{0}_A\right\rangle \otimes \left|\tilde{0}_B\right\rangle$, etc. Is our particular choice of $|\Psi_{AB}\rangle$ special in some way?

6.19.21 Matrix Representations

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ and $\{|0_B\rangle, |1_B\rangle\}$. Let $|0_A 0_B\rangle = |0_A\rangle \otimes |0_B\rangle$, etc. Let the natural tensor product basis kets for the joint space $\mathcal{H}_{AB}$ be represented by column vectors as follows:

$$|0_A 0_B\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \;,\; |0_A 1_B\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \;,\; |1_A 0_B\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \;,\; |1_A 1_B\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

For parts (a) -(c), let

$$\begin{aligned} \rho_{AB} = {} & \frac{3}{8} |0_A\rangle \langle 0_A| \otimes \frac{1}{2} (|0_B\rangle + |1_B\rangle) (|0_B\rangle + |1_B\rangle) \\ & + \frac{5}{8} |1_A\rangle \langle 1_A| \otimes \frac{1}{2} (|0_B\rangle - |1_B\rangle) (|0_B\rangle - |1_B\rangle) \end{aligned}$$

(a) Find the matrix representation of ρ_{AB} that corresponds to the above vector representation of the basis kets.

(b) Find the matrix representation of the partial projectors $I^A \otimes P_0^B$ and $I^A \otimes P_1^B$ 9see problem 6.18 for definitions) and then use them to compute the matrix representation of

$$\left(I^A \otimes P_0^B\right) \rho_{AB} \left(I^A \otimes P_0^B\right) + \left(I^A \otimes P_1^B\right) \rho_{AB} \left(I^A \otimes P_1^B\right)$$

(c) Find the matrix representation of $\tilde{\rho}_A = Tr_B[\rho_{AB}]$ by taking the partial trace using Dirac language methods.

6.19.22 Practice with Dirac Language for Joint Systems

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ and $\{|0_B\rangle, |1_B\rangle\}$. Let $|0_A 0_B\rangle = |0_A\rangle \otimes |0_B\rangle$, etc. Consider the joint state

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|0_A 0_B\rangle + |1_A 1_B\rangle)$$

(a) For this particular joint state, find the most general form of an observable O^A acting only on the A subsystem such that

$$\langle \Psi_{AB}| O^A \otimes I^B |\Psi_{AB}\rangle = \langle \Psi_{AB}| \left(I^A \otimes P_0^B\right) O^A \otimes I^B \left(I^A \otimes P_0^B\right) |\Psi_{AB}\rangle$$

where

$$P_0^B = \left|0^B\right\rangle \left\langle 0^B\right|$$

Express your answer in Dirac language.

(b) Consider the specific operator

$$X^A = \left|0^A\right\rangle \left\langle 1^A\right| + \left|1^A\right\rangle \left\langle 0^A\right|$$

which satisfies the general form you should have found in part (a). Find the most general form of the joint state vector $|\Psi'_{AB}\rangle$ such that

$$\langle\Psi'_{AB}| X^A \otimes I^B |\Psi'_{AB}\rangle \neq \langle\Psi_{AB}| \left(I^A \otimes P_0^B\right) X^A \otimes I^B \left(I^A \otimes P_0^B\right) |\Psi_{AB}\rangle$$

(c) Find an example of a reduced density matrix $\tilde{\rho}_A$ for the A subsystem such that no joint state vector $|\Psi'_{AB}\rangle$ of the general form you found in part (b) can satisfy

$$\tilde{\rho}_A = Tr_B \left[|\Psi'_{AB}\rangle \langle\Psi'_{AB}|\right]$$

6.19.23 More Mixed States

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ and $\{|0_B\rangle, |1_B\rangle\}$. Let $|0_A 0_B\rangle = |0_A\rangle \otimes |0_B\rangle$, etc. Suppose that both the A and B subsystems are initially under your control and you prepare the initial joint state

$$\left|\Psi_{AB}^0\right\rangle = \frac{1}{\sqrt{2}} \left(|0_A 0_B\rangle + |1_A 1_B\rangle\right)$$

(a) Suppose you take the A and B systems prepared in the state $\left|\Psi_{AB}^0\right\rangle$ and give them to your friend, who then performs the following procedure. Your friend flips a biased coin with probability p for heads; if the result of the coin-flip is a head your friend applies a transformation

$$U_h = |0_A 0_B\rangle \langle 0_A 0_B| - |1_A 1_B\rangle \langle 1_A 1_B|$$

If the result of the coin-flip is tails, your friend does nothing. After this procedure what is the density operator you should use to represent your knowledge of the joint state?

(b) Suppose you take the A and B systems prepared in the state $\left|\Psi_{AB}^0\right\rangle$ and give them to your friend, who then performs the alternate procedure. Your friend performs a measurement of the observable

$$O = I^A \otimes U_h$$

but does not tell you the result. After this procedure, what density operator should you use to represent your knowledge of the joint state? Assume that you can use the projection postulate (reduction) for state conditioning (preparation).

6.19.24 Complete Sets of Commuting Observables

Consider a three-dimensional Hilbert space $\mathcal{H}_3$ and the following set of operators:

$$O_\alpha \leftrightarrow \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \ , \ O_\beta \leftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \ , \ O_\gamma \leftrightarrow \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Find all possible complete sets of commuting observables(CSCO). That is, determine whether or not each of the sets

$$\{O_\alpha\}, \{O_\beta\}, \{O_\gamma\}, \{O_\alpha, O_\beta\}, \{O_\alpha, O_\gamma\}, \{O_\beta, O_\gamma\}, \{O_\alpha, O_\beta, O_\gamma\}$$

constitutes a valid CSCO.

6.19.25 Conserved Quantum Numbers

Determine which of the CSCO's in problem 6.24 (if any) are conserved by the Schrodinger equation with Hamiltonian

$$H = \varepsilon_0 \begin{pmatrix} 2 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \varepsilon_0 \left(O_\alpha\} + \{O_\beta\right)$$

Chapter 7

How Does It really Work: Photons, K-Mesons and Stern-Gerlach

7.5 Problems

7.5.1 Change the Basis

In examining light polarization in the text, we have been working in the $\{|x\rangle, |y\rangle\}$ basis.

(a) Just to show how easy it is to work in other bases, express $\{|x\rangle, |y\rangle\}$ in the $\{|R\rangle, |L\rangle\}$ and $\{|45^\circ\rangle, |135^\circ\rangle\}$ bases.

(b) If you are working in the $\{|R\rangle, |L\rangle\}$ basis, what would the operator representing a vertical polaroid look like?

7.5.2 Polaroids

Imagine a situation in which a photon in the $|x\rangle$ state strikes a vertically oriented polaroid. Clearly the probability of the photon getting through the vertically oriented polaroid is 0. Now consider the case of two polaroids with the photon in the $|x\rangle$ state striking a polaroid oriented at 45° and then striking a vertically oriented polaroid.

Show that the probability of the photon getting through both polaroids is $1/4$.

Consider now the case of three polaroids with the photon in the $|x\rangle$ state striking a polaroid oriented at 30° first, then a polaroid oriented at 60° and finally a vertically oriented polaroid.

Show that the probability of the photon getting through all three polaroids is $27/64$.

7.5.3 Calcite Crystal

A photon polarized at an angle θ to the optic axis is sent through a slab of calcite crystal. Assume that the slab is $10^{-2}\,cm$ thick, the direction of photon propagation is the $z-$axis and the optic axis lies in the $x-y$ plane.

Calculate, as a function of θ, he transition probability for the photon to emerge left circularly polarized. Sketch the result. Let the frequency of the light be given by $c/\omega = 5000\,\mathring{\mathrm{A}}$, and let $n_e = 1.50$ and $n_o = 1.65$ for the calcite indices of refraction.

7.5.4 Turpentine

Turpentine is an *optically active* substance. If we send plane polarized light into turpentine then it emerges with its plane of polarization rotated. Specifically, turpentine induces a left-hand rotation of about 5° per cm of turpentine that the light traverses. Write down the transition matrix that relates the incident polarization state to the emergent polarization state. Show that this matrix is unitary. Why is that important? Find its eigenvectors and eigenvalues, as a function of the length of turpentine traversed.

7.5.5 What QM is all about - Two Views

Photons polarized at 30° to the $x-$axis are sent through a $y-$polaroid. An attempt is made to determine how frequently the photons that pass through the polaroid, pass through as *right circularly polarized photons* and how frequently they pass through as *left circularly polarized photons*. This attempt is made as follows:

First, a prism that passes only right circularly polarized light is placed between the source of the 30° polarized photons and the $y-$polaroid, and it is determined how frequently the 30° polarized photons pass through the $y-$polaroid. Then this experiment is repeated with a prism that passes only left circularly polarized photons instead of the one that passes only right.

(a) Show by explicit calculation using standard amplitude mechanics that the sum of the probabilities for passing through the $y-$polaroid measured in these two experiments is different from the probability that one would measure if there were no prism in the path of the photon and only the $y-$polaroid.

Relate this experiment to the two-slit diffraction experiment.

(b) Repeat the calculation using density matrix methods instead of amplitude mechanics.

7.5.6 Photons and Polarizers

A photon polarization state for a photon propagating in the $z-$direction is given by

$$|\psi\rangle = \sqrt{\frac{2}{3}}\,|x\rangle + \frac{i}{\sqrt{3}}\,|y\rangle$$

(a) What is the probability that a photon in this state will pass through a polaroid with its transmission axis oriented in the $y-$direction?

(b) What is the probability that a photon in this state will pass through a polaroid with its transmission axis y' making an angle φ with the $y-$axis?

(c) A beam carrying N photons per second, each in the state $|\psi\rangle$, is totally absorbed by a black disk with its surface normal in the z-direction. How large is the torque exerted on the disk? In which direction does the disk rotate? **REMINDER**: The photon states $|R\rangle$ and $|L\rangle$ each carry a unit $\hbar$ of angular momentum parallel and antiparallel, respectively, to the direction of propagation of the photon.

7.5.7 Time Evolution

The matrix representation of the Hamiltonian for a photon propagating along the optic axis (taken to be the $z-$axis) of a quartz crystal using the linear polarization states $|x\rangle$ and $|y\rangle$ as a basis is given by

$$\hat{H} = \begin{pmatrix} 0 & -iE_0 \\ iE_0 & 0 \end{pmatrix}$$

(a) What are the eigenstates and eigenvalues of the Hamiltonian?

(b) A photon enters the crystal linearly polarized in the x direction, that is, $|\psi(0)\rangle = |x\rangle$. What is $|\psi(t)\rangle$, the state of the photon at time t? Express your answer in the $\{|x\rangle\,,|y\rangle\}$ basis.

(c) What is happening to the polarization of the photon as it travels through the crystal?

7.5.8 K-Meson oscillations

An additional effect to worry about when thinking about the time development of K-meson states is that the $|K_L\rangle$ and $|K_S\rangle$ states decay with time. Thus, we expect that these states should have the time dependence

$$|K_L(t)\rangle = e^{-i\omega_L t - t/2\tau_L}\,|K_L\rangle \quad , \quad |K_S(t)\rangle = e^{-i\omega_S t - t/2\tau_S}\,|K_S\rangle$$

where

$$\omega_L = E_L/\hbar \quad , \quad E_L = \left(p^2c^2 + m_L^2c^4\right)^{1/2}$$
$$\omega_S = E_S/\hbar \quad , \quad E_S = \left(p^2c^2 + m_S^2c^4\right)^{1/2}$$

and

$$\tau_S \approx 0.9 \times 10^{-10}\,\text{sec} \quad , \quad \tau_L \approx 560 \times 10^{-10}\,\text{sec}$$

Suppose that a pure K_L beam is sent through a thin absorber whose only effect is to change the relative phase of the K_0 and $\bar{K}_0$ amplitudes by $10°$. Calculate the number of K_S decays, relative to the incident number of particles, that will be observed in the first 5 cm after the absorber. Assume the particles have momentum $= mc$.

7.5.9 What comes out?

A beam of spin 1/2 particles is sent through series of three Stern-Gerlach measuring devices as shown in Figure 7.1 below: The first SGz device transmits

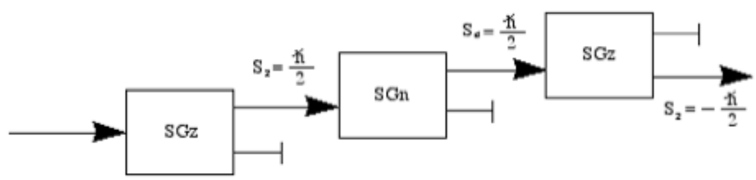

Figure 7.1: Stern-Gerlach Setup

particles with $\hat{S}_z = \hbar/2$ and filters out particles with $\hat{S}_z = -\hbar/2$. The second device, an SGn device transmits particles with $\hat{S}_n = \hbar/2$ and filters out particles with $\hat{S}_n = -\hbar/2$, where the axis $\hat{n}$ makes an angle θ in the $x - z$ plane with respect to the $z-$axis. Thus the particles passing through this SGn device are in the state

$$|+\hat{n}\rangle = \cos\frac{\theta}{2}\,|+\hat{z}\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|-\hat{z}\rangle$$

with the angle $\varphi = 0$. A last SGz device transmits particles with $\hat{S}_z = \hbar/2$ and filters out particles with $\hat{S}_z = -\hbar/2$.

(a) What fraction of the particles transmitted through the first SGz device will survive the third measurement?

(b) How must the angle θ of the SGn device be oriented so as to maximize the number of particles the at are transmitted by the final SGz device? What fraction of the particles survive the third measurement for this value of θ?

(c) What fraction of the particles survive the last measurement if the SGn device is simply removed from the experiment?

7.5.10 Orientations

The kets $|h\rangle$ and $|v\rangle$ are states of horizontal and vertical polarization, respectively. Consider the states

$$|\psi_1\rangle = -\frac{1}{2}\left(|h\rangle + \sqrt{3}\,|v\rangle\right) \quad , \quad |\psi_2\rangle = -\frac{1}{2}\left(|h\rangle - \sqrt{3}\,|v\rangle\right) \quad , \quad |\psi_2\rangle = |h\rangle$$

What are the relative orientations of the plane polarization for these three states?

7.5.11 Find the phase angle

If CP is not conserved in the decay of neutral K mesons, then the states of definite energy are no longer the K_L , K_S states, but are slightly different states $|K_L'\rangle$ and $|K_S'\rangle$. One can write, for example,

$$|K_L'\rangle = (1+\varepsilon)\left|K^0\right\rangle - (1-\varepsilon)\left|\bar{K}^0\right\rangle$$

where *varepsilon* is a very small complex number $\left(|\varepsilon| \approx 2\times 10^{-3}\right)$ that is a measure of the lack of CP conservation in the decays. The amplitude for a particle to be in $|K_L'\rangle$ (or $|K_S'\rangle$) varies as $e^{-i\omega_L t - t/2\tau_L}\left(or \quad e^{-i\omega_S t - t/2\tau_S}\right)$ where

$$\hbar\omega_L = \left(p^2c^2 + m_L^2c^4\right)^{1/2}\left(or \quad \hbar\omega_S = \left(p^2c^2 + m_S^2c^4\right)^{1/2}\right)$$

and $\tau_L \gg \tau_S$.

(a) Write out normalized expressions for the states $|K_L'\rangle$ and $|K_S'\rangle$ in terms of $|K_0\rangle$ and $\left|\bar{K}_0\right\rangle$.

(b) Calculate the ratio of the amplitude for a long-lived K to decay to two pions (a $CP = +1$ state) to the amplitude for a short-lived K to decay to two pions. What does a measurement of the ratio of these decay rates tell us about ε?

(c) Suppose that a beam of purely long-lived K mesons is sent through an absorber whose only effect is to change the relative phase of the K_0 and $\bar{K}_0$ components by δ. Derive an expression for the number of two pion events observed as a function of time of travel from the absorber. How well would such a measurement (given δ) enable one to determine the phase of ε?

7.5.12 Quarter-wave plate

A beam of linearly polarized light is incident on a quarter-wave plate (changes relative phase by 90°) with its direction of polarization oriented at 30° to the optic axis. Subsequently, the beam is absorbed by a black disk. Determine the rate angular momentum is transferred to the disk, assuming the beam carries N photons per second.

7.5.13 What is happening?

A system of N ideal linear polarizers is arranged in sequence. The transmission axis of the first polarizer makes an angle φ/N with the $y-$axis. The transmission axis of every other polarizer makes an angle φ/N with respect to the axis of the preceding polarizer. Thus, the transmission axis of the final polarizer makes an angle φ with the $y-$axis. A beam of $y-$polarized photons is incident on the first polarizer.

(a) What is the probability that an incident photon is transmitted by the array?

(b) Evaluate the probability of transmission in the limit of large N.

(c) Consider the special case with the angle 90°. Explain why your result is not in conflict with the fact that $\langle x \,|\, y \rangle = 0$.

7.5.14 Interference

Photons freely propagating through a vacuum have one value for their energy $E = h\nu$. This is therefore a $1-$dimensional quantum mechanical system, and since the energy of a freely propagating photon does not change, it must be an eigenstate of the energy operator. So, if the state of the photon at $t = 0$ is denoted as $|\psi(0)\rangle$, then the eigenstate equation can be written $\hat{H}\,|\psi(0)\rangle = E\,|\psi(0)\rangle$. To see what happens to the state of the photon with time, we simply have to apply the time evolution operator

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t)\,|\psi(0)\rangle = e^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle = e^{-ih\nu t/\hbar}\,|\psi(0)\rangle \\ &= e^{-i2\pi\nu t}\,|\psi(0)\rangle = e^{-i2\pi x/\lambda}\,|\psi(0)\rangle \end{aligned}$$

where the last expression uses the fact that $\nu = c/\lambda$ and that the distance it travels is $x = ct$. Notice that the relative probability of finding the photon at various points along the x-axis (the absolute probability depends on the number of photons emerging per unit time) does not change since the modulus-square of the factor in front of $|\psi(0)\rangle$ is 1. Consider the following situation. Two sources of identical photons face each other an emit photons at the same time. Let the distance between the two sources be L.

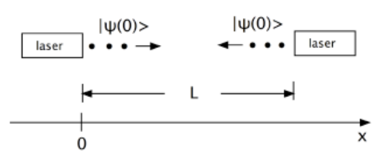

Figure 7.2: Interference Setup

Notice that we are assuming the photons emerge from each source in state $|\psi(0)\rangle$. In between the two light sources we can detect photons but we do not know from which source they originated. Therefore, we have to treat the photons at a point along the $x-$axis as a superposition of the time-evolved state from the left source and the time-evolved state from the right source.

(a) What is this superposition state $|\psi(t)\rangle$ at a point x between the sources? Assume the photons have wavelength λ.

(b) Find the relative probability of detecting a photon at point x by evaluating $|\langle\psi(t) \mid \psi(t)\rangle|^2$ at the point x.

(c) Describe in words what your result is telling you. Does this correspond to anything you have seen when light is described as a wave?

7.5.15 More Interference

Now let us tackle the two slit experiment with photons being shot at the slits one at a time. The situation looks something like the figure below. The distance between the slits, d is quite small (less than a mm) and the distance up the $y-$axis(screen) where the photons arrive is much,much less than L (the distance between the slits and the screen). In the figure, S_1 and S_2 are the lengths of the photon paths from the two slits to a point a distance y up the $y-$axis from the midpoint of the slits. The most important quantity is the difference in length between the two paths. The path length difference or PLD is shown in the figure.

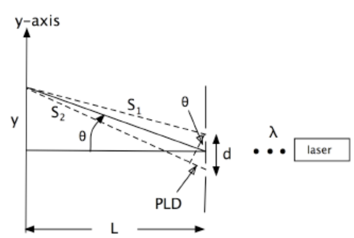

Figure 7.3: Double-Slit Interference Setup

We calculate PLD as follows:

$$PLD = d\sin\theta = d\left[\frac{y}{[L^2+y^2]^{1/2}}\right] \approx \frac{yd}{L} \quad , \quad y \ll L$$

Show that the relative probability of detecting a photon at various points along the screen is approximately equal to

$$4\cos^2\left(\frac{\pi y d}{\lambda L}\right)$$

7.5.16 The Mach-Zender Interferometer and Quantum Interference

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

Figure 7.4: Beam Splitter

output ports (see figure below), only one of them clicks. Which one clicks is completely random (that is, we have no better guess for one over the other). The input-output transformation of the waves incident on 50-50 beam splitters and perfectly reflecting mirrors are shown in the figure below.

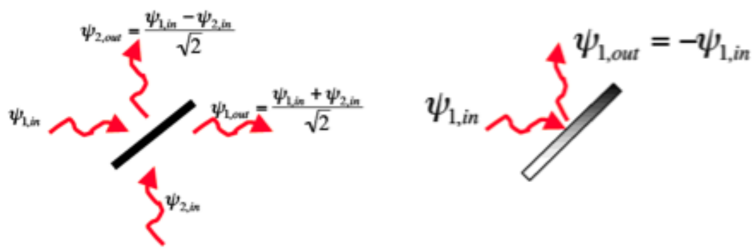

Figure 7.5: Input-Output transformation

(a) Show that with these rules, there is a 50-50 chance of either of the detectors shown in the first figure above to click.

(b) Now we set up a Mach-Zender interferometer(shown below):

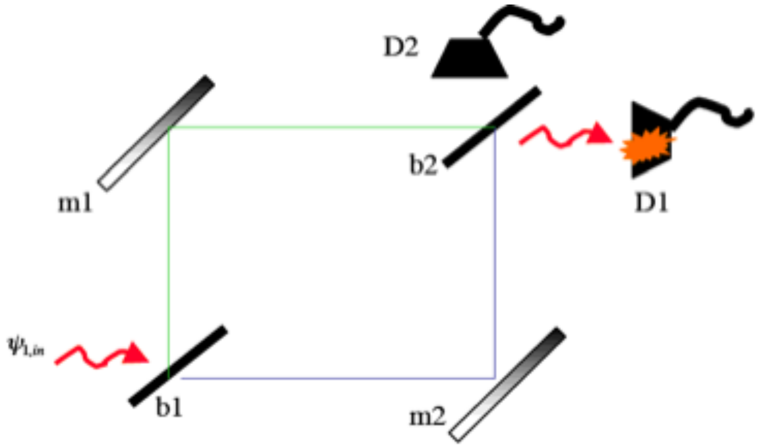

Figure 7.6: Input-Output transformation

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), show that the probability for detector D1 to click is 100% - *no randomness*!

(c) Classical logical reasoning would predict a probability for D1 to click given by

$$P_{D1} = P(transmission\ at\ b1|green\ path)P(green\ path) \\ + P(reflection\ at\ b2|blue\ path)P(blue\ path)$$

Calculate this and compare to the quantum result. *Explain*.

(d) 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.

7.5.17 More Mach-Zender

An experimenter sets up two optical devices for single photons. The first, (i) in figure below, is a standard balanced Mach-Zender interferometer with equal path lengths, perfectly reflecting mirrors (M) and 50-50 beam splitters (BS).

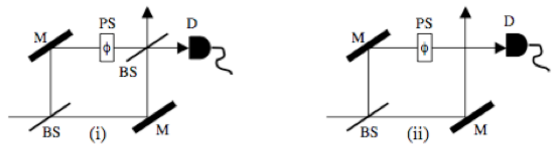

Figure 7.7: Mach-Zender Setups

A transparent piece of glass which imparts a phase shift (PS) ϕ is placed in one arm. Photons are detected (D) at one port. The second interferometer, (ii) in figure below, is the same *except* that the final beam splitter is omitted.

Sketch the probability of detecting the photon as a function of ϕ for each device. Explain your answer.

Chapter 8

Schrodinger Wave equation
1-Dimensional Quantum Systems

8.15 Problems

8.15.1 Delta function in a well

A particle of mass m moving in one dimension is confined to a space $0 < x < L$ by an infinite well potential. In addition, the particle experiences a delta function potential of strength λ given by $\lambda\delta(x - L/2)$ located at the center of the well as shown in Figure 8.1 below.

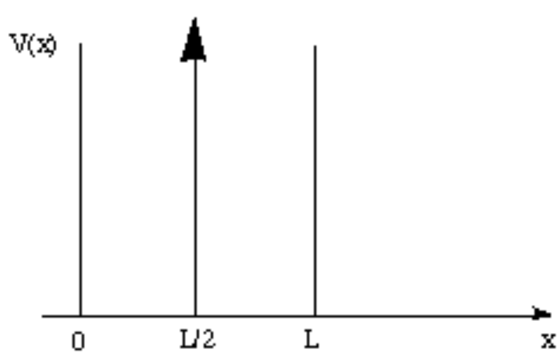

Figure 8.1: Potential Diagram

Find a transcendental equation for the energy eigenvalues E in terms of the mass m, the potential strength λ, and the size of the well L.

8.15.2 Properties of the wave function

A particle of mass m is confined to a one-dimensional region $0 \leq x \leq a$ (an infinite square well potential). At $t = 0$ its normalized wave function is

$$\psi(x, t = 0) = \sqrt{\frac{8}{5a}} \left(1 + \cos\left(\frac{\pi x}{a}\right)\right) \sin\left(\frac{\pi x}{a}\right)$$

(a) What is the wave function at a later time $t = t_0$?

(b) What is the average energy of the system at $t = 0$ and $t = t_0$?

(c) What is the probability that the particle is found in the left half of the box(i.e., in the region $0 \leq x \leq a/2$ at $t = t_0$?

8.15.3 Repulsive Potential

A repulsive short-range potential with a strongly attractive core can be approximated by a square barrier with a delta function at its center, namely,

$$V(x) = V_0 \Theta(x - |a|) - \frac{\hbar^2 g}{2m} \delta(x)$$

(a) Show that there is a negative energy eigenstate (the ground-state).

(b) If E_0 is the ground-state energy of the delta-function potential in the absence of the positive potential barrier, then the ground-state energy of the present system satisfies the relation $E \geq E_0 + V_0$. What is the particular value of V_0 for which we have the limiting case of a ground-state with zero energy.

8.15.4 Step and Delta Functions

Consider a one-dimensional potential with a step-function component and an attractive delta function component just at the edge of the step, namely,

$$V(x) = V \Theta(x) - \frac{\hbar^2 g}{2m} \delta(x)$$

(a) For $E > V$, compute the reflection coefficient for particle incident from the left. How does this result differ from that of the step barrier alone at high energy?

(b) For $E < 0$ determine the energy eigenvalues and eigenfunctions of any bound-state solutions.

8.15.5 Atomic Model

An approximate model for an atom near a wall is to consider a particle moving under the influence of the one-dimensional potential given by

$$V(x) = \begin{cases} -V_0\delta(x) & x > -d \\ \infty & x < -d \end{cases}$$

as shown in Figure 8.2 below.

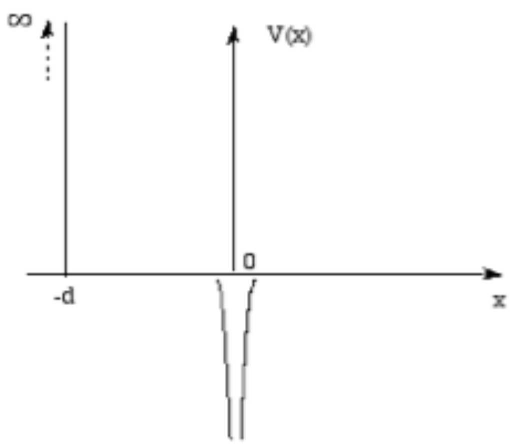

Figure 8.2: Potential Diagram

(a) Find the transcendental equation for the bound state energies.

(b) Find an approximation for the modification of the bound-state energy caused by the wall when it is *far away*. Define carefully what you mean by *far away*.

(c) What is the exact condition on V_0 and d for the existence of at least one bound state?

8.15.6 A confined particle

A particle of mass m is confined to a space $0 < x < a$ in one dimension by infinitely high walls at $x = 0$ and $x = a$. At $t = 0$ the particle is initially in the left half of the well with a wave function given by

$$\psi(x,0) = \begin{cases} \sqrt{2/a} & 0 < x < a/2 \\ 0 & a/2 < x < a \end{cases}$$

(a) Find the time-dependent wave function $\psi(x,t)$.

(b) What is the probability that the particle is in the n^{th} eigenstate of the well at time t?

(c) Derive an expression for average value of particle energy. What is the physical meaning of your result?

8.15.7 $1/x$ potential

An electron moves in one dimension and is confined to the right half-space $(x > 0)$ where it has potential energy

$$V(x) = -\frac{e^2}{4x}$$

where e is the charge on an electron.

(a) What is the solution of the Schrodinger equation at large x?

(b) What is the boundary condition at $x = 0$?

(c) Use the results of (a) and (b) to guess the ground state solution of the equation. Remember the ground state wave function has no zeros except at the boundaries.

(d) Find the ground state energy.

(e) Find the expectation value $\langle \hat{x} \rangle$ in the ground state.

8.15.8 Using the commutator

Using the coordinate-momentum commutation relation prove that

$$\sum_n (E_n - E_0) \left| \langle E_n | \hat{x} | E_0 \rangle \right|^2 = \text{constant}$$

where E_0 is the energy corresponding to the eigenstate $|E_0\rangle$. Determine the value of the constant. Assume the Hamiltonian has the general form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

8.15.9 Matrix Elements for Harmonic Oscillator

Compute the following matrix elements

$$\langle m | \hat{x}^3 | n \rangle \quad , \quad \langle m | \hat{x}\hat{p} | n \rangle$$

8.15.10 A matrix element

Show for the one dimensional simple harmonic oscillator

$$\langle 0| e^{ik\hat{x}} |0\rangle = \exp\left[-k^2 \langle 0| \hat{x}^2 |0\rangle /2\right]$$

where $\hat{x}$ is the position operator.

8.15.11 Correlation function

Consider a function, known as the *correlation function*, defined by

$$C(t) = \langle \hat{x}(t)\hat{x}(0)\rangle$$

where $\hat{x}(t)$ is the position operator in the Heisenberg picture. Evaluate the correlation function explicitly for the ground-state of the one dimensional simple harmonic oscillator.

8.15.12 Instantaneous Force

Consider a simple harmonic oscillator in its ground state.

An instantaneous force imparts momentum p_0 to the system such that the new state vector is given by

$$|\psi\rangle = e^{-ip_0\hat{x}/\hbar} |0\rangle$$

where $|0\rangle$ is the ground-state of the original oscillator.

What is the probability that the system will stay in its ground state?

8.15.13 Coherent States

Coherent states are defined to be eigenstates of the annihilation or lowering operator in the harmonic oscillator potential. Each coherent state has a complex label z and is given by $|z\rangle = e^{z\hat{a}^+} |0\rangle$.

(a) Show that $\hat{a}\,|z\rangle = z\,|z\rangle$

(b) Show that $\langle z_1 \mid z_2\rangle = e^{z_1^* z_2}$

(c) Show that the completeness relation takes the form

$$\hat{I} = \sum_n |n\rangle \langle n| = \int \frac{dxdy}{\pi} |z\rangle \langle z| \, e^{-z^* z}$$

where $|n\rangle$ is a standard harmonic oscillator energy eigenstate, $\hat{I}$ is the identity operator, $z = x + iy$, and the integration is taken over the whole $x-y$ plane(use polar coordinates).

8.15.14 Oscillator with Delta Function

Consider a harmonic oscillator potential with an extra delta function term at the origin, that is,

$$V(x) = \frac{1}{2}m\omega^2 x^2 + \frac{\hbar^2 g}{2m}\delta(x)$$

(a) Using the parity invariance of the Hamiltonian, show that the energy eigenfunctions are even and odd functions and that the simple harmonic oscillator odd-parity energy eigenstates are still eigenstates of the system Hamiltonian, with the same eigenvalues.

(b) Expand the even-parity eigenstates of the new system in terms of the even-parity harmonic oscillator eigenfunctions and determine the expansion coefficients.

(c) Show that the energy eigenvalues that correspond to even eigenstates are solutions of the equation

(d)

$$\frac{2}{g} = -\sqrt{\frac{\hbar}{m\pi\omega}}\sum_{k=0}^{\infty}\frac{(2k)!}{2^{2k}(k!)^2}\left(2k+\frac{1}{2}-\frac{E}{\hbar\omega}\right)^{-1}$$

You might need the fact that

$$\psi_{2k}(0) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{\sqrt{(2k)!}}{2^k k!}$$

Consider the following cases:

(1) $g > 0$, $E > 0$

(2) $g < 0$, $E > 0$

(3) $g < 0$, $E < 0$

Show the first and second cases correspond to an infinite number of energy eigenvalues.

Where are they relative to the original energy eigenvalues of the harmonic oscillator?

Show that in the third case, that of an attractive delta function core, there exists a single eigenvalue corresponding to the ground state of the system provided that the coupling is such that

$$\left[\frac{\Gamma(3/4)}{\Gamma(1/4)}\right]^2 < \frac{g^2\hbar}{16m\omega} < 1$$

You might need the series summation:

$$\sum_{k=0}^{\infty} \frac{(2k)!}{4^k (k!)^2} \frac{1}{2k+1-x} = \frac{\sqrt{\pi}}{2} \frac{\Gamma(1/2 - x/2)}{\Gamma(1 - x/2)}$$

You will need to look up other properties of the gamma function to solve this problem.

8.15.15 Measurement on a Particle in a Box

Consider a particle in a box of width a, prepared in the ground state.

(a) What are then possible values one can measure for: (1) energy, (2) position, (3) momentum ?

(b) What are the probabilities for the possible outcomes you found in part (a)?

(c) At some time (call it t = 0) we perform a measurement of position. However, our detector has only finite resolution. We find that the particle is in the middle of the box (call it the origin) with an uncertainty $\Delta x = a/2$, that is, we know the position is, for sure, in the range $-a/4 < x < a/4$, but we are completely uncertain where it is within this range. What is the (normalized) post-measurement state?

(d) Immediately after the position measurement what are the possible values for (1) energy, (2) position, (3) momentum and with what probabilities?

(e) At a later time, what are the possible values for (1) energy, (2) position, (3) momentum and with what probabilities? Comment.

8.15.16 Aharonov-Bohm experiment

Consider an infinitely long solenoid which carries a current I so that there is a constant magnetic field inside the solenoid(see Figue 8.3 below).

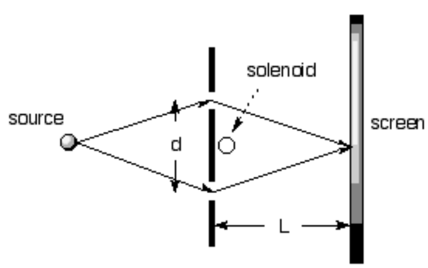

Figure 8.3: Aharonov-Bohm Setup

Suppose that in the region outside the solenoid the motion of a particle with charge e and mass m is described by the Schrodinger equation. Assume that for $I = 0$, the solution of the equation is given by

$$\psi_0(\vec{r}, t) = e^{iE_0 t/\hbar}\psi_0(\vec{r})$$

(a) Write down and solve the Schrodinger equation in the region outside the solenoid in the case $I \neq 0$.

(b) Consider the two-slit diffraction experiment for the particles described above shown in Figure 8.3 above. Assume that the distance d between the two slits is large compared to the diameter of the solenoid.

Compute the shift ΔS of the diffraction pattern on the screen due to the presence of the solenoid with $I \neq 0$. Assume that $L \gg \Delta S$.

8.15.17 A Josephson Junction

A Josephson junction is formed when two superconducting wires are separated by an insulating gap of capacitance C. The quantum states ψ_i , $i = 1, 2$ of the two wires can be characterized by the numbers n_i of Cooper pairs (charge $=$ $-2e$) and phases θ_i, such that $\psi_i = \sqrt{n_i}e^{i\theta_i}$ (Ginzburg-Landau approximation). The (small) amplitude that a pair tunnel across a narrow insulating barrier is $-E_J/n_0$ where $n_0 = n_1 + n_2$ and E_J is the the so-called Josephson energy. The interesting physics is expressed in terms of the differences

$$n = n_2 - n_1 \quad , \quad \varphi = \theta_2 - \theta_1$$

We consider a junction where

$$n_1 \approx n_2 \approx n_0/2$$

When there exists a nonzero difference n between the numbers of pairs of charge $-2e$, where $e > 0$, on the two sides of the junction, there is net charge $-ne$ on side 2 and net charge $+ne$ on side 1. Hence a voltage difference ne/C arises, where the voltage on side 1 is higher than that on side 2 if $n = n_2 - n_1 > 0$. Taking the zero of the voltage to be at the center of the junction, the electrostatic energy of the Cooper pair of charge $-2e$ on side 2 is ne^2/C, and that of a pair on side 1 is $-ne^2/C$. The total electrostatic energy is $C(\Delta V)^2/2 = Q^2/2C = (ne)^2/2C$.

The equations of motion for a pair in the two-state system $(1, 2)$ are

$$\begin{aligned} i\hbar\frac{d\psi_1}{dt} &= U_1\psi_1 - \frac{E_J}{n_0}\psi_2 = -\frac{ne^2}{C}\psi_1 - \frac{E_J}{n_0}\psi_2 \\ i\hbar\frac{d\psi_2}{dt} &= U_2\psi_2 - \frac{E_J}{n_0}\psi_1 = \frac{ne^2}{C}\psi_2 - \frac{E_J}{n_0}\psi_1 \end{aligned}$$

(a) Discuss the physics of the terms in these equations.

(b) Using $\psi_i = \sqrt{n_i}e^{i\theta_i}$, show that the equations of motion for n and φ are given by

$$\dot{\varphi} = \dot{\theta}_2 - \dot{\theta}_1 \approx -\frac{2ne^2}{\hbar C}$$
$$\dot{n} = \dot{n}_2 - \dot{n}_1 \approx \frac{E_J}{\hbar}\sin\varphi$$

(c) Show that the pair(electric current) from side 1 to side 2 is given by

$$J_S = J_0 \sin\varphi \quad , \quad J_0 = \frac{\pi E_J}{\phi_0}$$

(d) Show that

$$\ddot{\varphi} \approx -\frac{2e^2 E_J}{\hbar^2 C}\sin\varphi$$

For E_J positive, show that this implies there are oscillations about $\varphi = 0$ whose angular frequency (called the Josephson plasma frequency)is given by

$$\omega_J = \sqrt{\frac{2e^2 E_J}{\hbar^2 C}}$$

for small amplitudes.

If E_J is negative, then there are oscillations about $\varphi = \pi$.

(e) If a voltage $V = V_1 - V_2$ is applied across the junction(by a battery), a charge $Q_1 = VC = (-2e)(-n/2) = en$ is held on side 1, and the negative of this on side 2. Show that we then have

$$\dot{\varphi} \approx -\frac{2eV}{\hbar} \equiv -\omega$$

which gives $\varphi = \omega t$.

The battery holds the charge difference across the junction fixed at $VC - en$, but can be a source or sink of charge such that a current can flow in the circuit. Show that in this case, the current is given by

$$J_S = -J_0 \sin\omega t$$

i.e., the DC voltage of the battery generates an AC pair current in circuit of frequency

$$\omega = \frac{2eV}{\hbar}$$

8.15.18 Eigenstates using Coherent States

Obtain eigenstates of the following Hamiltonian

$$\hat{H} = \hbar\omega\hat{(a)}^{+}\hat{a} + V\hat{a} + V^{*}\hat{a}^{+}$$

for a complex V using coherent states.

8.15.19 Bogliubov Transformation

Suppose annihilation and creation operators satisfy the standard commutation relations $[\hat{a}, \hat{a}^{+}] = 1$. Show that the Bogliubov transformation

$$\hat{b} = \hat{a}\cosh\eta + \hat{a}^{+}\sinh\eta$$

preserves the commutation relation of the creation and annihilation operators, i.e., $[\hat{b}, \hat{b}^{+}] = 1$. Use this fact to obtain eigenvalues of the following Hamiltonian

$$\hat{H} = \hbar\omega\hat{(a)}^{+}\hat{a} + \frac{1}{2}V\left(\hat{a}\hat{a} + \hat{a}^{+}\hat{a}^{+}\right)$$

(There is an upper limit on V for which this can be done). Also show that the unitary operator

$$\hat{U} = e^{\left(\hat{a}\hat{a}+\hat{a}^{+}\hat{a}^{+}\right)\eta/2}$$

can relate the two sets of operators as $\hat{b} = \hat{U}\hat{a}\hat{U}^{-1}$.

8.15.20 Harmonic oscillator

Consider a particle in a 1−dimensional harmonic oscillator potential. Suppose at time $t = 0$, the state vector is

$$|\psi(0)\rangle = e^{-\frac{i\hat{p}a}{\hbar}}|0\rangle$$

where $\hat{p}$ is the momentum operator and a is a real number.

(a) Use the equation of motion in the Heisenberg picture to find the operator $\hat{x}(t)$.

(b) Show that $e^{-\frac{i\hat{p}a}{\hbar}}$ is the translation operator.

(c) In the Heisenberg picture calculate the expectation value $\langle x\rangle$ for $t \geq 0$.

8.15.21 Another oscillator

A 1−dimensional harmonic oscillator is, at time $t = 0$, in the state

$$|\psi(t=0)\rangle = \frac{1}{\sqrt{3}}\left(|0\rangle + |1\rangle + |2\rangle\right)$$

where $|n\rangle$ is the n^{th} energy eigenstate. Find the expectation value of position and energy at time t.

8.15.22 The coherent state

Consider a particle of mass m in a harmonic oscillator potential of frequency ω. Suppose the particle is in the state

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$$

where

$$c_n = e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}}$$

and α is a complex number. As we have discussed, this is a *coherent state* or alternatively a *quasi-classical state.*

(a) Show that $|\alpha\rangle$ is an eigenstate of the annihilation operator, i.e., $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$.

(b) Show that in this state $\langle\hat{x}\rangle = x_c \mathrm{Re}(\alpha)$ and $\langle\hat{p}\rangle = p_c \mathrm{Im}(\alpha)$. Determine x_c and p_c.

(c) Show that, in position space, the wave function for this state is $\psi_\alpha(x) = e^{ip_0x/\hbar}u_0(x - x_0)$ where $u_0(x)$ is the ground state gaussian function and $\langle\hat{x}\rangle = x_0$ and $\langle\hat{p}\rangle = p_0$.

(d) What is the wave function in momentum space? Interpret x_0 and p_0.

(e) Explicitly show that $\psi_\alpha(x)$ is an eigenstate of the annihilation operator using the position-space representation of the annihilation operator.

(f) Show that the coherent state is a minimum uncertainty state (with equal uncertainties in x and p, in characteristic dimensionless units.

(g) If a time $t = 0$ the state is $|\psi(0)\rangle = |\alpha\rangle$, show that at a later time,

$$|\psi(t)\rangle = e^{-i\omega t/2} \left|\alpha e^{-i\omega t}\right\rangle$$

Interpret this result.

(h) Show that, as a function of time, $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ follow the classical trajectory of the harmonic oscillator, hence the name *quasi-classical* state.

(i) Write the wave function as a function of time, $\psi_\alpha(x,t)$. Sketch the time evolving probability density.

(j) Show that in the classical limit

$$\lim_{|\alpha|\to\infty} \frac{\Delta N}{\langle N\rangle} \to 0$$

(k) Show that the probability distribution in n is Poissonian, with appropriate parameters.

(l) Use a *rough* time-energy uncertainty principle , to find an uncertainty principle $\Delta E \Delta t > \hbar$ between the number and phase of a quantum oscillator.

8.15.23 Neutrino Oscillations

It is generally recognized that there are at least three different kinds of neutrinos. They can be distinguished by the reactions in which the neutrinos are created or absorbed. Let us call these three types of neutrino ν_e, ν_μ and ν_τ. It has been speculated that each of these neutrinos has a small but finite rest mass, possibly different for each type. Let us suppose, for this exam question, that there is a small perturbing interaction between these neutrino types, in the absence of which all three types of neutrinos have the same nonzero rest mass M_0. The Hamiltonian of the system can be written as

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

where

$$\hat{H}_0 = \begin{pmatrix} M_0 & 0 & 0 \\ 0 & M_0 & 0 \\ 0 & 0 & M_0 \end{pmatrix} \rightarrow \text{ no interactions present}$$

and

$$\hat{H}_1 = \begin{pmatrix} 0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & 0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & 0 \end{pmatrix} \rightarrow \text{ effect of interactions}$$

where we have used the basis

$$|\nu_e\rangle = |1\rangle \quad , \quad |\nu_\mu\rangle = |2\rangle \quad , \quad |\nu_\tau\rangle = |3\rangle$$

(a) First assume that $\omega_1 = 0$, i.e., no interactions. What is the time development operator? Discuss what happens if the neutrino initially was in the state

$$|\psi(0)\rangle = |\nu_e\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \text{ or } |\psi(0)\rangle = |\nu_\mu\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ or } |\psi(0)\rangle = |\nu_\tau\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

What is happening physically in this case?

(b) Now assume that $\omega_1 \neq 0$, i.e., interactions are present. Also assume that at $t = 0$ the neutrino is in the state

$$|\psi(0)\rangle = |\nu_e\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

What is the probability as a function of time, that the neutrino will be in each of the other two states?

(c) An experiment to detect the *neutrino oscillations* is being performed. The flight path of the neutrinos is 2000 meters. Their energy is $100\,GeV$. The sensitivity of the experiment is such that the presence of 1% of neutrinos different from those present at the start of the flight can be measured with confidence. Let $M_0 = 20\,eV$. What is the smallest value of $\hbar\omega_1$ that can be detected? How does this depend on M_0? Don't ignore special relativity.

8.15.24 Generating Function

Use the generating function for Hermite polynomials

$$e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

to work out the matrix elements of x in the position representation, that is, compute

$$\langle x \rangle_{nn'} = \int_{-\infty}^{\infty} \psi_n^*(x) x \psi_{n'}(x) dx$$

where

$$\psi_n(x) = N_n H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}$$

and

$$N_n = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!}\right)^{1/2} \quad , \quad \alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}$$

8.15.25 Given the wave function ......

A particle of mass m moves in one dimension under the influence of a potential $V(x)$. Suppose it is in an energy eigenstate

$$\psi(x) = \left(\frac{\gamma^2}{\pi}\right)^{1/4} \exp\left(-\gamma^2 x^2/2\right)$$

with energy $E = \hbar^2\gamma^2/2m$.

(a) Find the mean position of the particle.

(b) Find the mean momentum of the particle.

(c) Find $V(x)$.

(d) Find the probability $P(p)dp$ that the particle's momentum is between p and $p + dp$.

8.15.26 What is the oscillator doing?

Consider a one dimensional simple harmonic oscillator. Use the number basis to do the following algebraically:

(a) Construct a linear combination of $|0\rangle$ and $|1\rangle$ such that $\langle \hat{x} \rangle$ is as large as possible.

(b) Suppose the oscillator is in the state constructed in (a) at $t = 0$. What is the state vector for $t > 0$? Evaluate the expectation value $\langle \hat{x} \rangle$ as a function of time for $t > 0$ using (i)the Schrodinger picture and (ii) the Heisenberg picture.

(c) Evaluate $\left\langle (\Delta x)^2 \right\rangle$ as a function of time using either picture.

8.15.27 Coupled oscillators

Two identical harmonic oscillators in one dimension each have a mass m and frequency ω. Let the two oscillators be coupled by an interaction term Cx_1x_2 where C is a constant and x_1 and x_2 are the coordinates of the two oscillators. Find the exact energy spectrum of eigenvalues for this coupled system.

8.15.28 Interesting operators ....

The operator $\hat{c}$ is defined by the following relations:

$$\hat{c}^2 = 0 \quad , \quad \hat{c}\hat{c}^+ + \hat{c}^+\hat{c} = \left\{\hat{c}, \hat{c}^+\right\} = \hat{I}$$

(a) Show that

1. $\hat{N} = \hat{c}^+\hat{c}$ is Hermitian
2. $\hat{N}^2 = \hat{N}$
3. The eigenvalues of $\hat{N}$ are 0 and 1 (eigenstates $|0\rangle$ and $|1\rangle$)
4. $\hat{c}^+ |0\rangle = |1\rangle \quad , \quad \hat{c}\,|0\rangle = 0$

(b) Consider the Hamiltonian

$$\hat{H} = \hbar\omega_0(\hat{c}^+\hat{c} + 1/2)$$

Denoting the eigenstates of $\hat{H}$ by $|n\rangle$, show that the only nonvanishing states are the states $|0\rangle$ and $|1\rangle$ defined in (a).

(c) Can you think of any physical situation that might be described by these new operators?

8.15.29 What is the state?

A particle of mass m in a one dimensional harmonic oscillator potential is in a state for which a measurement of the energy yields the values $\hbar\omega/2$ or $3\hbar\omega/2$, each with a probability of one-half. The average value of the momentum $\langle \hat{p}_x \rangle$ at time $t = 0$ is $(m\omega\hbar/2)^{1/2}$. This information specifies the state of the particle completely. What is this state and what is $\langle \hat{p}_x \rangle$ at time t?

8.15.30 Things about particle in box

A particle of mass m moves in a one-dimensional box Infinite well) of length ℓ with the potential

$$V(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 < x < \ell \\ \infty & x > \ell \end{cases}$$

At $t = 0$, the wave function of this particle is known to have the form

$$\psi(x,0) = \begin{cases} \sqrt{30/\ell^5}\,x(\ell - x) & 0 < x < \ell \\ 0 & \text{otherwise} \end{cases}$$

(a) Write this wave function as a linear combination of energy eigenfunctions

$$\psi_n(x) = \sqrt{\frac{2}{\ell}}\sin\left(\frac{\pi n x}{\ell}\right) \quad , \quad E_n = n^2\frac{\pi^2\hbar^2}{2m\ell^2} \quad , \quad n = 1,2,3,....$$

(b) What is the probability of measuring E_n at $t = 0$?

(c) What is $\psi(x, t > 0)$?

8.15.31 Handling arbitrary barriers.....

Electrons in a metal are bound by a potential that may be approximated by a finite square well. Electrons fill up the energy levels of this well up to an energy called the *Fermi energy* as shown in the figure below:

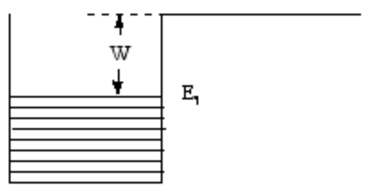

Figure 8.4: Finite Square Well

The difference between the Fermi energy and the top of the well is the *work function* W of the metal. Photons with energies exceeding the work function can eject electrons from the metal - this is the so-called *photoelectric effect*.

Another way to pull out electrons is through application of an external uniform electric field $\vec{\mathcal{E}}$, which alters the potential energy as shown in the figure below:

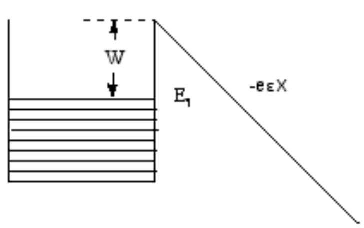

Figure 8.5: Finite Square Well + Electric Field

?By approximating (see notes below) the linear part of the function by a series of square barriers, show that the transmission coefficient for electrons at the Fermi energy is given by

$$T \approx \exp\left(\frac{-4\sqrt{2m}W^{3/2}}{3e\left|\vec{\varepsilon}\right|\hbar}\right)$$

How would you expect this *field- or cold-emission* current to vary with the applied voltage? As part of your problem solution explain the method.

This calculation also plays a role in the derivation of the current-voltage characteristic of a Schottky diode in semiconductor physics.

Approximating an Arbitrary Barrier

For a rectangular barrier of width a and height V_0, we found the transmission coefficient

$$T = \frac{1}{1+\frac{V_0^2\sinh^2\gamma a}{4E(V_0-E)}}, \gamma^2 = (V_0-E)\frac{2m}{\hbar^2}, k^2 = \frac{2m}{\hbar^2}E$$

A useful limiting case occurs for $\gamma a \gg 1$. In this case

$$\sinh\gamma a = \frac{e^{\gamma a}-e^{-\gamma a}}{2} \underset{\gamma a>>1}{\rightarrow} \frac{e^{\gamma a}}{2}$$

so that

$$T = \frac{1}{1+\left(\frac{\gamma^2+k^2}{4k\gamma}\right)^2\sinh^2\gamma a} \underset{\gamma a>>1}{\rightarrow} \left(\frac{4k\gamma}{\gamma^2+k^2}\right)^2 e^{-2\gamma a}$$

Now if we evaluate the natural log of the transmission coefficient we find

$$\ln T \underset{\gamma a>>1}{\rightarrow} \ln\left(\frac{4k\gamma}{\gamma^2+k^2}\right)^2 - 2\gamma a \underset{\gamma a\gg 1}{\rightarrow} -2\gamma a$$

where we have dropped the logarithm relative to γa since $\ln(almost\,anything)$ is not very large. This corresponds to only including the exponential term.

We can now use this result to calculate the probability of transmission through a non-square barrier, such as that shown in the figure below:

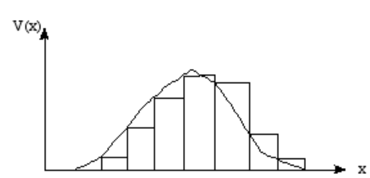

Figure 8.6: Arbitrary Barrier Potential

When we only include the exponential term, the probability of transmission through an arbitrary barrier, as above, is just the product of the individual transmission coefficients of a succession of rectangular barrier as shown above. Thus, if the barrier is sufficiently smooth so that we can approximate it by a series of rectangular barriers (each of width Δx) that are not too thin for the condition $\gamma a \gg 1$ to hold, then for the barrier as a whole

$$\ln T \approx \ln \prod_i T_i = \sum_i \ln T_i = -2 \sum_i \gamma_i \Delta x$$

If we now assume that we can approximate this last term by an integral, we find

$$T \approx \exp\left(-2 \sum_i \gamma_i \Delta x\right) \approx \exp\left(-2 \int \sqrt{\frac{2m}{\hbar^2}} \sqrt{V(x) - E} dx\right)$$

where the integration is over the region for which the square root is real.

You may have a somewhat uneasy feeling about this crude derivation. Clearly, the approximations made break down near the turning points, where $E = V(x)$. Nevertheless, a more detailed treatment shows that it works amazingly well.

8.15.32 Deuteron model

Consider the motion of a particle of mass $m = 0.8 \times 10^{-24}\, gm$ in the well shown in the figure below:

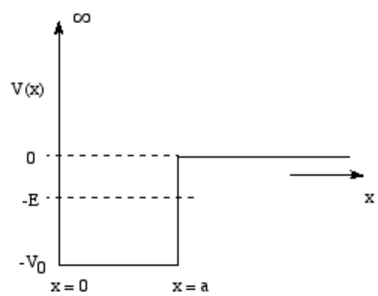

Figure 8.7: Deuteron Model

The size of the well (range of the potential) is $a = 1.4 \times 10^{-13}\, cm$. If the binding energy of the system is $2.2\, MeV$, find the depth of the potential V_0 in MeV. This is a model of the deuteron in one dimension.

8.15.33 Use Matrix Methods

A one-dimensional potential barrier is shown in the figure below.
Define and calculate the transmission probability for a particle of mass m and

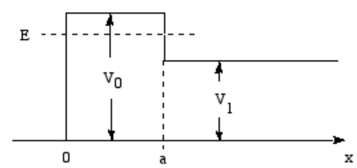

Figure 8.8: A Potential Barrier

energy E ($V_1 < E < V_0$) incident on the barrier from the left. If you let $V_1 \to 0$ and $a \to 2a$, then you can compare your answer to other textbook results. Develop matrix methods (as in the text) to solve the boundary condition equations.

8.15.34 Finite Square Well Encore

Consider the symmetric finite square well of depth V_0 and width a.

(a) Let $k_0 = sqrt2mV_0/\hbar^2$. Sketch the bound states for the following choices of $k_0a/2$.

(i) $\frac{k_0a}{2} = 1$, $(ii)\frac{k_0a}{2} = 1.6$, $(iii)\frac{k_0a}{2} = 5$

(b) Show that no matter how shallow the well, there is at least one bound state of this potential. Describe it.

(c) Let us re-derive the bound state energy for the delta function well directly from the limit of the the finite potential well. Use the graphical solution discussed in the text. Take the limit as $a \to 0$, $V_0 \to \infty$, but $aV_0 \to U_0$(constant) and show that the binding energy is $E_b = mU_0^2/2\hbar^2$.

(d) Consider now the half-infinite well, half-finite potential well as shown below.

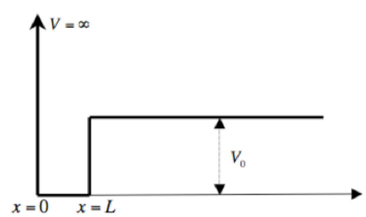

Figure 8.9: Half-Infinite, Half-Finite Well

Without doing any calculation, show that there are no bound states unless $k_0L > \pi/2$. HINT: think about erecting an infinite wall down the center of a symmetric finite well of width $a = 2L$. Also, think about parity.

(e) Show that in general, the binding energy eigenvalues satisfy the eigenvalue equation

$$\kappa = -k \cot kL$$

where

$$\kappa = \sqrt{\frac{2mE_b}{\hbar^2}} \quad and \quad k^2 + \kappa^2 = k_0^2$$

8.15.35 Half-Infinite Half-Finite Square Well Encore

Consider the unbound case ($E > V_0$) eigenstate of the potential below.

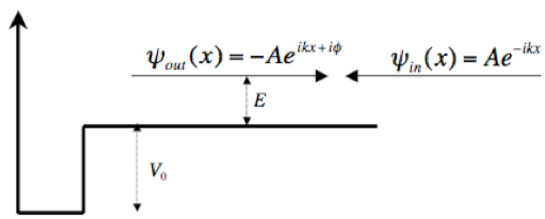

Figure 8.10: Half-Infinite, Half-Finite Well Again

Unlike the potentials with finite wall, the scattering in this case has only one output channel - reflection. If we send in a plane wave towards the potential, $\psi_{in}(x) = Ae^{-ikx}$, where the particle has energy $E = (\hbar k)^2/2m$, the reflected wave will emerge from the potential with a phase shift, $\psi_{out}(x) = Ae^{ikx+\phi}$,

(a) Show that the reflected wave is phase shifted by

$$\phi = 2\tan^{-1}\left(\frac{k}{q}\tan qL\right) - 2kL$$

where

$$q^2 = k^2 + k_0^2 \quad , \quad \frac{\hbar^2 k_0^2}{2m} = V_0$$

(b) Plot the function of ϕ as a function of $k_0 L$ for fixed energy. Comment on your plot.

(c) The phase shifted reflected wave is equivalent to that which would arise from a hard wall, but moved a distance L' from the origin.

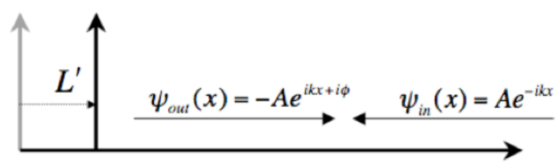

Figure 8.11: Shifted Wall

What is the effective L' as a function of the phase shift ϕ induced by our semi-finite well? What is the maximum value of L'? Can L' be negative? From your plot in (b), sketch L' as a function of $k_0 L$, for fixed energy. Comment on your plot.

8.15.36 Nuclear α Decay

Nuclear *alpha*−decays $(A, Z) \to (A-2, Z-2) + \alpha$ have lifetimes ranging from nanoseconds (or shorter) to millions of years (or longer). This enormous range was understood by George Gamov by the exponential sensitivity to underlying parameters in tunneling phenomena. Consider $\alpha = {}^4He$ as a point particle in the potential given schematically in the figure below.
The potential barrier is due to the Coulomb potential $2(Z-2)e^2/r$. The probability of tunneling is proportional to the so-called Gamov's transmission coefficients obtained in Problem 8.31

$$T = exp\left[-\frac{2}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}\,dx\right]$$

where a and b are the classical turning points (where $E = V(x)$) Work out numerically T for the following parameters: $Z = 92$ (Uranium), size of nucleus

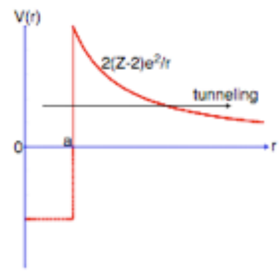

Figure 8.12: Nuclear Potential Model

$a = 5\,fm$ and the kinetic energy of the α particle $1\,MeV$, $3\,MeV$, $10\,MeV$, $30\,MeV$.

8.15.37 One Particle, Two Boxes

Consider two boxes in 1-dimension of width a, with infinitely high walls, separated by a distance $L = 2a$. We define the box by the potential energy function sketched below.

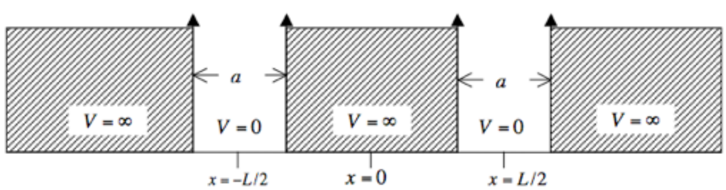

Figure 8.13: Two Boxes

A particle experiences this potential and its state is described by a wave function. The energy eigenfunctions are *doubly* degenerate, $\left\{\phi_n^{(+)}, \phi_n^{(-)} \,|\, n = 1, 2, 3, 4, ...\right\}$ so that

$$E_n^{(+)} = E_n^{(-)} = n^2 \frac{\pi^2 \hbar^2}{2ma^2}$$

where $\phi_n^{(\pm)} = u_n(x \pm L/2)$ with

$$u_n(x) = \begin{cases} \sqrt{2/a}\cos\left(\frac{n\pi x}{a}\right) \,,\; n = 1, 3, 5, ... & -a/2 < x < a/2 \\ \sqrt{2/a}\sin\left(\frac{n\pi x}{a}\right) \,,\; n = 2, 4, 6, ... & -a/2 < x < a/2 \\ 0 & |x| > a/2 \end{cases}$$

Suppose at time $t = 0$ the wave function is

$$\psi(x) = \frac{1}{2}\phi_1^{(-)}(x) + \frac{1}{2}\phi_2^{(-)}(x) \tag{8.1}$$

At this time, answer parts (a) - (c)

(a) What is the probability of finding the particle in the state $\phi_1^{(+)}(x)$?

(b) What is the probability of finding the particle with energy $\pi^2\hbar^2/2ma^2$?

(c) CLAIM: At $t = 0$ there is a 50-50 chance for finding the particle in either box. Justify this claim.

(d) What is the state at a later time assuming no measurements are done?

Now let us generalize. Suppose we have an arbitrary wave function at $t = 0$, $\psi(x, 0)$, that satisfies all the boundary conditions.

(e) Show that, in general, the probability to find the particle in the left box does not change with time. Explain why this makes sense physically.

Switch gears again ......

(f) Show that the state $\Phi_n(x) = c_1\phi_n^{(+)}(x) + c_2\phi_n^{(-)}(x)$ (where c_1 and c_2 are arbitrary complex numbers) is a stationary state.

Consider then the state described by the wave function $\psi(x) = (\phi_1^{(+)}(x) + c_2\phi_1^{(-)}(x))/\sqrt{2}$.

(g) Sketch the probability density in x. What is the mean value $\langle x \rangle$? How does this change with time?

(h) Show that the momentum space wave function is

$$\tilde{\psi}(p) = \sqrt{2}\cos\left(pL/2\hbar\right)\tilde{u}_1(p)$$

where

$$\tilde{u}_1(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} u_1(x)e^{-ipx/\hbar}$$

is the momentum-space wave function of $u_1(x)$.

(i) Without calculation, what is the mean value $\langle p \rangle$? How does this change with time?

(j) Suppose the potential energy was somehow *turned off* (don't ask me how, just imagine it was done) so the particle is now free.

Without doing any calculation, sketch how you expect the position-space wave function to evolve at later times, showing all important features. Please explain your sketch.

8.15.38 A half-infinite/half-leaky box

Consider a one dimensional potential

$$V(x) = \begin{cases} \infty & x < 0 \\ U_0\delta(x-a) & x > 0 \end{cases}$$

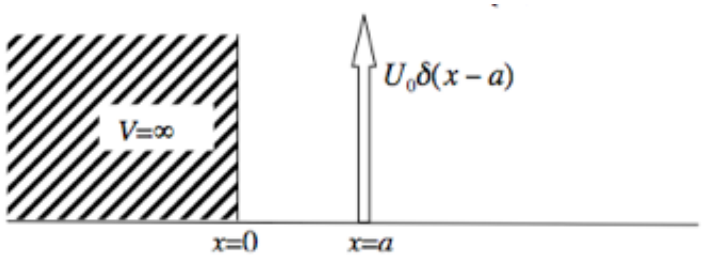

Figure 8.14: Infinite Wall + Delta Function

(a) Show that the stationary states with energy E can be written

$$u(x) = \begin{cases} 0 & x < 0 \\ A\frac{\sin(ka+\phi(k))}{\sin(ka)}\sin(kx) & 0 < x < a \\ A\sin(kx+\phi(k)) & x > a \end{cases}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad , \quad \phi(k) = \tan^{-1}\left[\frac{k\tan(ka)}{k-\gamma_0\tan(ka)}\right] \quad , \quad \gamma_0 = \frac{2mU_0}{\hbar^2}$$

What is the nature of these states - bound or unbound?

(b) Show that the limits $\gamma_0 \to 0$ and $\gamma_0 \to \infty$ give reasonable solutions.

(c) Sketch the energy eigenfunction when $ka = \pi$. Explain this solution.

(d) Sketch the energy eigenfunction when $ka = \pi/2$. How does the probability to find the particle in the region $0 < x < a$ compare with that found in part (c)? Comment.

(e) In a scattering scenario, we imagine sending in an incident plane wave which is reflected with unit probabiklity, but phase shifted according to the conventios shown in the figure below:
Show that the phase shift of the scattered wave is $\delta(k) = 2\phi(k)$.

There exist mathematical conditions such that the so-called *S-matrix element* $e^{i\delta(k)}$ blows up. For these solutions is k real, imaginary, or complex? Comment.

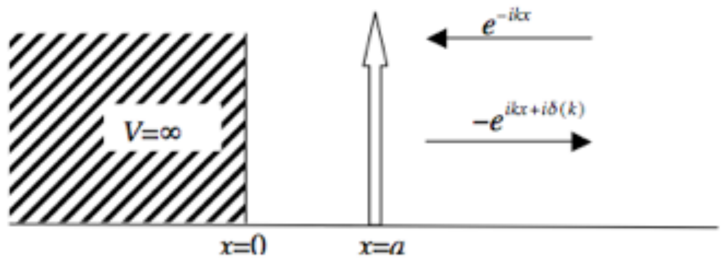

Figure 8.15: Scattering Scenario

8.15.39 Neutrino Oscillations Redux

Read the article T. Araki *et al*, "Measurement of Neutrino Oscillations with Kam LAND: Evidence of Spectral Distortion," *Phys. Rev. Lett.* **94**, 081801 (2005), which shows the neutrino oscillation, a quantum phenomenon demonstrated at the largest distance scale yet (about 180 km).

(a) The Hamiltonian for an ultrarelativistic particle is approximated by

$$H = \sqrt{p^2c^2 + m^2c^4} \approx pc + \frac{m^2c^3}{2p}$$

for p=$|\vec{p}|$. Suppose in a basis of two states, m^2 is given as a 2×2 matrix

$$m^2 = m_0^2 I + \frac{\Delta m^2}{2}\begin{pmatrix} -\cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & \cos(2\theta) \end{pmatrix}$$

Write down the eigenstates of m^2.

(b) Calculate the probability for the state

$$|\psi\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

to be still found in the same state after time interval t for definite momentum p.

(c) Using the data shown in Fig. 3 of the article, estimate approximately values of Δm^2 and $\sin^2 2\theta$.

8.15.40 Is it in the ground state?

An infinitely deep one-dimensional potential well runs fro $x = 0$ to $x = a$. The normalized energy eigenstates are

$$u_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad , \quad n = 1, 2, 3, ...$$

A particle is placed in the left-hand half of the well so that its wavefunction is $\psi =$ constant for $x < a/2$. If the energy of the particle is now measured, what is the probability of finding it in the ground state?

8.15.41 Some Thoughts on T-Violation

Any Hamiltonian can be recast to the form

$$H = U \begin{pmatrix} E_1 & 0 & \dots & 0 \\ 0 & E_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & E_n \end{pmatrix} U^+$$

where U is a general $n \times n$ unitary matrix.

(a) Show that the time evolution operator is given by

$$e^{-iHt/\hbar} = U \begin{pmatrix} e^{-iE_1 t/\hbar} & 0 & \dots & 0 \\ 0 & e^{-iE_2 t/\hbar} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & e^{-iE_n t/\hbar} \end{pmatrix} U^+$$

(b) For a two-state problem, the most general unitary matrix is

$$U = e^{i\theta} \begin{pmatrix} \cos\theta e^{i\phi} & -\sin\theta e^{i\eta} \\ \sin\theta e^{-i\eta} & \cos\theta e^{-i\phi} \end{pmatrix}$$

Work out the probabilities $P(1 \to 2)$ and $P(2 \to 1)$ over time interval t and verify that they are the same despite the the apparent T-violation due to complex phases. NOTE: This is the same problem as the neutrino oscillation (problem 8.39) if you set $E_i = \sqrt{p^2c^2 + m^2c^4} \approx pc + \frac{m^2c^3}{2p}$ and set all phases to zero.

(c) For a three-state problem, however, the time-reversal invariance can be broken. Calculate the difference $P(1 \to 2) - P(2 \to 1)$ for the following form of the unitary matrix

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta} \\ 0 & 1 & 0 \\ -s_{13}e^{i\delta} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where five unimportant phases have been dropped. The notation is $s_{12} = \sin\theta_{12}, c_{23} = \cos\theta_{23}$, etc.

(d) For CP-conjugate states (e.g.., anti-neutrinos($\bar{\nu}$) vs neutrinos(ν), the Hamiltonian is given by substituting U^* in place of U. Show that the probabilities $P(1 \to 2)$ and $P(\bar{1} \to \bar{2})$ can differ (CP violation) yet CPT is respected, ie., $P(1 \to 2) = P(\bar{2} \to \bar{1})$.

8.15.42 Kronig-Penney Model

Consider a periodic repulsive potential of the form

$$V = \sum_{n=-\infty}^{\infty} \lambda\delta(x - na)$$

with $\lambda > 0$. The general solution for $-a < x < 0$ is given by

$$\psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x}$$

with $\kappa = \sqrt{2mE}/\hbar$. Using Bloch's theorem, the wave function for the next period $0 < x < a$ is given by

$$\psi(x) = e^{ika}\left(Ae^{i\kappa(x-a)} + Be^{-i\kappa(x-a)}\right)$$

for $|k| \leq \pi/a$. Answer the following questions.

(a) Write down the continuity condition for the wave function and the required discontinuity for its derivative at $x = 0$. Show that the phase e^{ika} under the discrete translation $x \to x + a$ is given by κ as

$$e^{ika} = \cos\kappa a + \frac{1}{\kappa d}\sin\kappa a \pm i\sqrt{1 - \left(\cos\kappa a + \frac{1}{\kappa d}\sin\kappa a\right)^2}$$

Here and below, $d = \hbar^2/m\lambda$.

(b) Take the limit of zero potential $d \to \infty$ and show that there are no gaps between the bands as expected for a free particle.

(c) When the potential is weak but finite (lartge d) show analytically that there appear gaps between the bands at $k = \pm\pi/a$.

(d) Plot the relationship between κ and k for a weak potential ($d = 3a$) and a strong potential ($d = a/3$) (both solutions together).

(e) You always find two values of k at the same energy (or κ). What discrete symmetry guarantees this degeneracy?

8.15.43 Operator Moments and Uncertainty

Consider an observable O_A for a finite-dimensional quantum system with spectral decomposition

$$O_A = \sum_i \lambda_i P_i$$

(a) Show that the exponential operator $E_A = exp(O_A)$ has spectral decomposition

$$E_A = \sum_i e^{\lambda_i P_i}$$

Do this by inserting the spectral decomposition of O_A into the power series expansion of the exponential.

(b) Prove that for any state $|\Psi_A\rangle$ such that $\Delta O_A = 0$, we automatically have $\Delta E_A = 0$.

8.15.44 Uncertainty and Dynamics

Consider the observable

$$O_X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and the initial state

$$|\Psi_A(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

(a) Compute the uncertainty $\Delta O_X = 0$ with respect to the initial state $|\Psi_A(0)\rangle$.

(b) Now let the state evolve according to the Schrodinger equation, with Hamiltonian operator

$$H = \hbar \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

Compute the uncertainty $\Delta O_X = 0$ as a function of t.

(c) Repeat part (b) but replace O_X with the observable

$$O_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

That is, compute the uncertainty ΔO_Z as a function of t assuming evolution according to the Schrodinger equation with the Hamiltonian above.

(d) Show that your answers to parts (b) and (c) always respect the Heisenberg Uncertainty Relation

$$\Delta O_X \Delta O_Z \geq \frac{1}{2} |\langle [O_X, O_Z] \rangle|$$

Are there any times t at which the Heisenberg Uncertainty Relation is satisfied with equality?

Chapter 9

Angular Momentum; 2- and 3-Dimensions

9.7 Problems

9.7.1 Position representation wave function

A system is found in the state

$$\psi(\theta, \varphi) = \sqrt{\frac{15}{8\pi}} \cos\theta \sin\theta \cos\varphi$$

(a) What are the possible values of $\hat{L}_z$ that measurement will give and with what probabilities?

(b) Determine the expectation value of $\hat{L}_x$ in this state.

9.7.2 Operator identities

Show that

(a) $\left[\vec{a} \cdot \vec{L}, \vec{b} \cdot \vec{L}\right] = i\hbar \left(\vec{a} \times \vec{b}\right) \cdot \vec{L}$ holds under the assumption that $\vec{a}$ and $\vec{b}$ commute with each other and with $\vec{L}$.

(b) for any vector operator $\vec{V}(\hat{x}, \hat{p})$ we have $\left[\vec{L}^2, \vec{V}\right] = 2i\hbar \left(\vec{V} \times \vec{L} - i\hbar\vec{V}\right)$.

9.7.3 More operator identities

Prove the identities

(a) $\left(\vec{\sigma} \cdot \vec{A}\right)\left(\vec{\sigma} \cdot \vec{B}\right) = \vec{A} \cdot \vec{B} + i\vec{\sigma} \cdot \left(\vec{A} \times \vec{B}\right)$

(b) $e^{i\phi\vec{S}\cdot\hat{n}/\hbar}\vec{\sigma}e^{-i\phi\vec{S}\cdot\hat{n}/\hbar} = \hat{n}(\hat{n} \cdot \vec{\sigma}) + \hat{n} \times [\hat{n} \times \vec{\sigma}] \cos\phi + [\hat{n} \times \vec{\sigma}] \sin\phi$

9.7.4 On a circle

Consider a particle of mass μ constrained to move on a circle of radius a. Show that

$$H = \frac{L^2}{2\mu a^2}$$

Solve the eigenvalue/eigenvector problem of H and interpret the degeneracy.

9.7.5 Rigid rotator

A rigid rotator is immersed in a uniform magnetic field $\vec{B} = B_0 \hat{e}_z$ so that the Hamiltonian is

$$\hat{H} = \frac{\hat{L}^2}{2I} + \omega_0 \hat{L}_z$$

where ω_0 is a constant. If

$$\langle \theta, \phi \mid \psi(0) \rangle = \sqrt{\frac{3}{4\pi}} \sin\theta \sin\phi$$

what is $\langle \theta, \phi \mid \psi(t) \rangle$? What is $\left\langle \hat{L}_x \right\rangle$ at time t?

9.7.6 A Wave Function

A particle is described by the wave function

$$\psi(\rho, \phi) = A e^{-\rho^2/2\Delta} \cos^2 \phi$$

Determine $P(L_z = 0)$, $P(L_z = 2\hbar)$ and $P(L_z = -2\hbar)$.

9.7.7 $L = 1$ System

Consider the following operators on a 3-dimensional Hilbert space

$$L_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \; L_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad , \; L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(a) What are the possible values one can obtain if L_z is measured?

(b) Take the state in which $L_z = 1$. In this state, what are $\langle L_x \rangle$, $\left\langle L_x^2 \right\rangle$ and $\Delta L_x = \sqrt{\langle L_x^2 \rangle - \langle L_x \rangle^2}$.

(c) Find the normalized eigenstates and eigenvalues of L_x in the L_z basis.

(d) If the particle is in the state with $L_z = -1$ and L_x is measured, what are the possible outcomes and their probabilities?

(e) Consider the state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1 \end{pmatrix}$$

in the L_z basis. If L_z^2 is measured and a result $+1$ is obtained, what is the state after the measurement? How probable was this result? If L_z is measured, what are the outcomes and respective probabilities?

(f) A particle is in a state for which the probabilities are $P(L_z = 1) = 1/4$, $P(L_z = 0) = 1/2$ and $P(L_z = -1) = 1/4$. Convince yourself that the most general, normalized state with this property is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2} |L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}} |L_z = 0\rangle + \frac{e^{i\delta_3}}{2} |L_z = -1\rangle$$

We know that if $|\psi\rangle$ is a normalized state then the state $e^{i\theta} |\psi\rangle$ is a physically equivalent state. Does this mean that the factors $e^{i\delta_j}$ multiplying the L_z eigenstates are irrelevant? Calculate, for example, $P(L_x = 0)$.

9.7.8 A Spin-3/2 Particle

Consider a particle with spin angular momentum $j = 3/2$. The are four sublevels with this value of j, but different eigenvalues of j_z, $|m = 3/2\rangle$,$|m = 1/2\rangle$,$|m = -1/2\rangle$ and $|m = -3/2\rangle$.

(a) Show that the *raising operator* in this 4−dimensional space is

$$\hat{j}_+ = \hbar \left(\sqrt{3} \, |3/2\rangle \langle 1/2| + 2 \, |1/2\rangle \langle -1/2| + \sqrt{3} \, |-1/2\rangle \langle -3/2| \right)$$

where the states have been labeled by the j_z quantum number.

(b) What is the lowering operator $\hat{j}_-$?

(c) What are the matrix representations of $\hat{J}_\pm$, $\hat{J}_x$, $\hat{J}_y$, $\hat{J}_z$ and $\hat{J}^2$ in the j_z basis?

(d) Check that the state

$$|\psi\rangle = \frac{1}{2\sqrt{2}} \left(\sqrt{3} \, |3/2\rangle + |1/2\rangle - |-1/2\rangle - \sqrt{3} \, |-3/2\rangle \right)$$

is an eigenstate of $\hat{J}_x$ with eigenvalue $\hbar/2$.

(e) Find the eigenstate of $\hat{J}_x$ with eigenvalue $3\hbar/2$.

(f) Suppose the particle describes the nucleus of an atom, which has a magnetic moment described by the operator $\vec{\mu} = g_N \mu_N \vec{j}$, where g_N is the *g-factor* and μ_N is the so-called *nuclear magneton*. At time $t = 0$, the system is prepared in the state given in (c). A magnetic field, pointing in the y direction of magnitude B, is suddenly turned on. What is the evolution of $\left\langle \hat{j}_z \right\rangle$ as a function of time if

$$\hat{H} = -\hat{\mu} \cdot \vec{B} = -g_N \mu_N \hbar \vec{J} \cdot \vec{B}\hat{y} = -g_N \mu_N \hbar B \hat{J}_y$$

where $\mu_N = e\hbar/2Mc$ = nuclear magneton? You will need to use the identity we derived earlier

$$e^{x\hat{A}} \hat{B} e^{-x\hat{A}} = \hat{B} + \left[\hat{A}, \hat{B}\right] x + \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] \frac{x^2}{2} + \left[\hat{A}, \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right]\right] \frac{x^3}{6} + ...$$

9.7.9 Arbitrary directions

Method #1

(a) Using the $|z+\rangle$ and $|z-\rangle$ states of a spin 1/2 particle as a basis, set up and solve as a problem in matrix mechanics the eigenvalue/eigenvector problem for $S_n = \vec{S} \cdot \hat{n}$ where the spin operator is

$$\vec{S} = \hat{S}_x \hat{e}_x + \hat{S}_y \hat{e}_y + \hat{S}_z \hat{e}_z$$

and

$$\hat{n} = \sin\theta \cos\varphi \hat{e}_x + \sin\theta \sin\varphi \hat{e}_y + \cos\theta \hat{e}_z$$

(b) Show that the eigenstates may be written as

$$|\hat{n}+\rangle = \cos\frac{\theta}{2} |z+\rangle + e^{i\varphi} \sin\frac{\theta}{2} |z-\rangle$$
$$|\hat{n}-\rangle = \sin\frac{\theta}{2} |z+\rangle - e^{i\varphi} \cos\frac{\theta}{2} |z-\rangle$$

Method #2

This part demonstrates another way to determine the eigenstates of $S_n = \vec{S} \cdot \hat{n}$.

The operator

$$\hat{R}(\theta \hat{e}_y) = e^{-i\hat{S}_y \theta/\hbar}$$

rotates spin states by an angle θ counterclockwise about the $y-$axis.

(a) Show that this rotation operator can be expressed in the form

$$\hat{R}(\theta \hat{e}_y) = \cos\frac{\theta}{2} - \frac{2i}{\hbar} \hat{S}_y \sin\frac{\theta}{2}$$

(b) Apply $\hat{R}$ to the states $|z+\rangle$ and $|z-\rangle$ to obtain the state $|\hat{n}+\rangle$ with $varphi =$ 0, that is, rotated by angle θ in the $x - z$ plane.

9.7.10 Spin state probabilities

The z-component of the spin of an electron is measured and found to be $+\hbar/2$.

(a) If a subsequent measurement is made of the $x-$component of the spin, what are the possible results?

(b) What are the probabilities of finding these various results?

(c) If the axis defining the measured spin direction makes an angle θ with respect to the original $z-$axis, what are the probabilities of various possible results?

(d) What is the expectation value of the spin measurement in (c)?

9.7.11 A spin operator

Consider a system consisting of a spin 1/2 particle.

(a) What are the eigenvalues and normalized eigenvectors of the operator

$$\hat{Q} = A\hat{s}_y + B\hat{s}_z$$

where $\hat{s}_y$ and $\hat{s}_z$ are spin angular momentum operators and A and B are real constants.

(b) Assume that the system is in a state corresponding to the larger eigenvalue. What is the probability that a measurement of $\hat{s}_y$ will yield the value $+\hbar/2$?

9.7.12 Simultaneous Measurement

A beam of particles is subject to a simultaneous measurement of the angular momentum observables $\hat{L}^2$ and $\hat{L}_z$. The measurement gives pairs of values

$$(\ell, m) = (0, 0) \quad and \quad (1, -1)$$

with probabilities 3/4 and 1/4 respectively.

(a) Reconstruct the state of the beam immediately before the measurements.

(b) The particles in the beam with $(\ell, m) = (1, -1)$ are separated out and subjected to a measurement of $\hat{L}_x$. What are the possible outcomes and their probabilities?

(c) Construct the spatial wave functions of the states that could arise from the second measurement.

9.7.13 Vector Operator

Consider a vector operator $\vec{V}$ that satisfies the commutation relation

$$[L_i, V_j] = i\hbar\varepsilon_{ijk}V_k$$

This is the definition of a *vector operator*.

(a) Prove that the operator $e^{-i\varphi L_x/\hbar}$ is a rotation operator corresponding to a rotation around the $x-$axis by an angle φ, by showing that

$$e^{-i\varphi L_x/\hbar}V_i e^{i\varphi L_x/\hbar} = R_{ij}(\varphi)V_j$$

where $R_{ij}(\varphi)$ is the corresponding rotation matrix.

(b) Prove that

$$e^{-i\varphi L_x}|\ell, m\rangle = |\ell, -m\rangle$$

(c) Show that a rotation by π around the $z-$axis can also be achieved by first rotating around the $x-$axis by $\pi/2$, then rotating around the $y-$axis by π and, finally rotating back by $-\pi/2$ around the $x-$axis. In terms of rotation operators this is expressed by

$$e^{i\pi L_x/2\hbar}e^{-i\pi L_y/\hbar}e^{-i\pi L_x/2\hbar} = e^{-i\pi L_z/\hbar}$$

9.7.14 Addition of Angular Momentum

Two atoms with $J_1 = 1$ and $J_2 = 2$ are coupled, with an energy described by $\hat{H} = \varepsilon\vec{J}_1 \cdot \vec{J}_2$, $\varepsilon > 0$. Determine all of the energies and degeneracies for the coupled system.

9.7.15 Spin $= 1$ system

We now consider a spin $= 1$ system.

(a) Use the spin $= 1$ states $|1,1\rangle$, $|1,0\rangle$ and $|1,-1\rangle$ (eigenstates of $\hat{S}_z$) as a basis to form the matrix representation (3×3) of the angular momentum operators $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$, $\hat{S}^2$, $\hat{S}_+$, and $\hat{S}_-$.

(b) Determine the eigenstates of $\hat{S}_x$ in terms of the eigenstates $|1,1\rangle$, $|1,0\rangle$ and $|1,-1\rangle$ of $\hat{S}_z$.

(c) A spin $= 1$ particle is in the state

$$|\psi\rangle = \frac{1}{\sqrt{14}}\begin{pmatrix} 1 \\ 2 \\ 3i \end{pmatrix}$$

in the $\hat{S}_z$ basis.

(1) What are the probabilities that a measurement of $\hat{S}_z$ will yield the values $\hbar$, 0, or $-\hbar$ for this state? What is $\left\langle \hat{S}_z \right\rangle$?

(2) What is $\left\langle \hat{S}_x \right\rangle$ in this state?

(3) What is the probability that a measurement of $\hat{S}_x$ will yield the value $\hbar$ for this state?

(d) A particle with spin = 1 has the Hamiltonian

$$\hat{H} = A\hat{S}_z + \frac{B}{\hbar}\hat{S}_x^2$$

(1) Calculate the energy levels of this system.

(2) If, at $t = 0$, the system is in an eigenstate of $\hat{S}_x$ with eigenvalue $\hbar$, calculate the expectation value of the spin $\left\langle \hat{S}_Z \right\rangle$ at time t.

9.7.16 Deuterium Atom

Consider a deuterium atom (composed of a nucleus of spin = 1 and an electron). The electronic angular momentum is $\vec{J} = \vec{L} + \vec{S}$, where $\vec{L}$ is the orbital angular momentum of the electron and $\vec{S}$ is its spin. The total angular momentum of the atom is $\vec{F} = \vec{J} + \vec{I}$, where $\vec{I}$ is the nuclear spin. The eigenvalues of $\hat{J}^2$ and $\hat{F}^2$ are $J(J+1)\hbar^2$ and $F(F+1)\hbar^2$ respectively.

(a) What are the possible values of the quantum numbers J and F for the deuterium atom in the $1s(L = 0)$ ground state?

(b) What are the possible values of the quantum numbers J and F for a deuterium atom in the $2p(L = 1)$ excited state?

9.7.17 Spherical Harmonics

Consider a particle in a state described by

$$\psi = N(x + y + 2z)e^{-\alpha r}$$

where N is a normalization factor.

(a) Show, by rewriting the $Y_1^{\pm1,0}$ functions in terms of x, y, z and r that

$$Y_1^{\pm1} = \mp\left(\frac{3}{4\pi}\right)^{1/2}\frac{x \pm iy}{\sqrt{2}r} \quad , \quad Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\frac{z}{r}$$

(b) Using this result, show that for a particle described by ψ above

$$P(L_z = 0) = 2/3\ ,\ P(L_z = \hbar) = 1/6\ ,\ P(L_z = -\hbar) = 1/6$$

9.7.18 Spin in Magnetic Field

Suppose that we have a spin$-1/2$ particle interacting with a magnetic field via the Hamiltonian

$$\hat{H} = \begin{cases} -\vec{\mu}\cdot\vec{B} \ , \ \vec{B} = B\hat{e}_z & 0 \leq t < T \\ -\vec{\mu}\cdot\vec{B} \ , \ \vec{B} = B\hat{e}_y & T \leq t < 2T \end{cases}$$

where $\vec{\mu} = \mu_B\vec{\sigma}$ and the system is initially($t = 0$) in the state

$$|\psi(0)\rangle = |x+\rangle = \frac{1}{\sqrt{2}}\left(|z+\rangle + |z-\rangle\right)$$

Determine the probability that the state of the system at $t = 2T$ is

$$|\psi(2T)\rangle = |x+\rangle$$

in three ways:

(1) Using the Schrodinger equation (solving differential equations)

(2) Using the time development operator (using operator algebra)

(3) Using the density operator formalism

9.7.19 What happens in the Stern-Gerlach box?

An atom with spin $= 1/2$ passes through a Stern-Gerlach apparatus adjusted so as to transmit atoms that have their spins in the $+z$ direction. The atom spends time T in a magnetic field B in the $x-$direction.

(a) At the end of this time what is the probability that the atom would pass through a Stern-Gerlach selector for spins in the $-z$ direction?

(b) Can this probability be made equal to one, if so, how?

9.7.20 Spin = 1 particle in a magnetic field

[Use the results from Problem 9.15]. A particle with intrinsic spin = 1 is placed in a uniform magnetic field $\vec{B} = B_0\hat{e}_x$. The initial spin state is $|\psi(0)\rangle = |1,1\rangle$. Take the spin Hamiltonian to be $\hat{H} = \omega_0\hat{S}_x$ and determine the probability that the particle is in the state $|\psi(t)\rangle = |1,-1\rangle$ at time t.

9.7.21 Multiple magnetic fields

A spin$-1/2$ system with magnetic moment $\vec{\mu} = \mu_0\vec{\sigma}$ is located in a uniform time-independent magnetic field B_0 in the positive $z-$direction. For the time interval $0 < t < T$ an additional uniform time-independent field B_1 is applied in the positive $x-$direction. During this interval, the system is again in a uniform constant magnetic field, but of different magnitude and direction z' from the initial one. At and before $t = 0$, the system is in the $m = 1/2$ state with respect to the $z-$axis.

(a) At $t = 0+$, what are the amplitudes for finding the system with spin projections $m' = 1/2$ with respect to the $z'-$axis?

(b) What is the time development of the energy eigenstates with respect to the z' direction, during the time interval $0 < t < T$?

(c) What is the probability at $t = T$ of observing the system in the spin state $m = -1/2$ along the original $z-$axis? [Express answers in terms of the angle θ between the z and z' axes and the frequency $\omega_0 = \mu_0 B_0/\hbar$]

9.7.22 Neutron interferometer

In a classic table-top experiment (neutron interferometer), a monochromatic neutron beam ($\lambda = 1.445\mathring{A}$) is split by Bragg reflection at point A of an interferometer into two beams which are then recombined (after another reflection) at point D as in Figure 9.1 below:

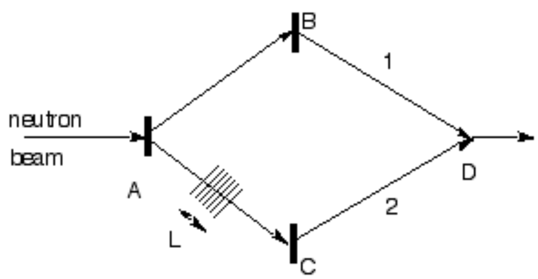

Figure 9.1: Neutron Interferometer Setup

One beam passes through a region of transverse magnetic field of strength B (direction shown by lines)for a distance L. Assume that the two paths from A to D are identical except for the region of magnetic field.

(a) Find the explicit expression for the dependence of the intensity at point D on B, L and the neutron wavelength, with the neutron polarized parallel or anti-parallel to the magnetic field.

(b) Show that the change in the magnetic field that produces two successive maxima in the counting rates is given by

$$\Delta B = \frac{8\pi^2 \hbar c}{|e|\, g_n \lambda L}$$

where g_n $(= -1.91)$ is the neutron magnetic moment in units of $-e\hbar/2m_n c$. This calculation was a PRL publication in 1967.

9.7.23 Magnetic Resonance

A particle of spin 1/2 and magnetic moment μ is placed in a magnetic field $\vec{B} = B_0\hat{z} + B_1\hat{x}\cos\omega t - B_1\hat{y}\sin\omega t$, which is often employed in magnetic resonance experiments. Assume that the particle has spin up along the $+z-$axis at $t = 0$ ($m_z = +1/2$). Derive the probability to find the particle with spin down ($m_z = -1/2$) at time $t > 0$.

9.7.24 More addition of angular momentum

Consider a system of two particles with $j_1 = 2$ and $j_2 = 1$. Determine the $|j, m, j_1, j_2\rangle$ states listed below in the $|j_1, m_1, j_2, m_2\rangle$ basis.

$$|3,3,j_1,j_2\rangle \ , \ |3,2,j_1,j_2\rangle \ , \ |3,1,j_1,j_2\rangle \ , \ |2,2,j_1,j_2\rangle \ , \ |2,1,j_1,j_2\rangle \ , \ |1,1,j_1,j_2\rangle$$

9.7.25 Clebsch-Gordan Coefficients

Work out the Clebsch-Gordan coefficients for the combination

$$\frac{3}{2} \otimes \frac{1}{2}$$

9.7.26 Spin$-1/2$ and Density Matrices

Let us consider the application of the density matrix formalism to the problem of a spin$-1/2$ particle in a static external magnetic field. In general, a particle with spin may carry a magnetic moment, oriented along the spin direction (by symmetry). For spin$-1/2$, we have that the magnetic moment (operator) is thus of the form:

$$\hat{\mu}_i = \frac{1}{2}\gamma\hat{\sigma}_i$$

where the $\hat{\sigma}_i$ are the Pauli matrices and γ is a constant giving the strength of the moment, called the gyromagnetic ratio. The term in the Hamiltonian for such a magnetic moment in an external magnetic field, $\vec{B}$ is just:

$$\hat{H} = -\vec{\mu} \cdot \vec{B}$$

The spin$-1/2$ particle has a spin orientation or *polarization* given by

$$\vec{P} = \langle\vec{\sigma}\rangle$$

Let us investigate the motion of the polarization vector in the external field. Recall that the expectation value of an operator may be computed from the density matrix according to

$$\left\langle \hat{A} \right\rangle = Tr\left(\hat{\rho}\hat{A}\right)$$

In addition the time evolution of the density matrix is given by

$$i\frac{\partial\hat{\rho}}{\partial t} = \left[\hat{H}(t), \hat{\rho}(t)\right]$$

Determine the time evolution $d\vec{P}/dt$ of the polarization vector. Do not make any assumption concerning the purity of the state. Discuss the physics involved in your results.

9.7.27 System of N Spin$-1/2$ Particle

Let us consider a system of N spin$-1/2$ particles per unit volume in thermal equilibrium, in an external magnetic field $\vec{B}$. In thermal equilibrium the canonical distribution applies and we have the density operator given by:

$$\hat{\rho} = \frac{e^{-\hat{H}t}}{Z}$$

where Z is the partition function given by

$$Z = Tr\left(e^{-\hat{H}t}\right)$$

Such a system of particles will tend to orient along the magnetic field, resulting in a bulk magnetization (having units of magnetic moment per unit volume), $\vec{M}$.

(a) Give an expression for this magnetization $\vec{M} = N\gamma\langle\vec{\sigma}/2\rangle$(dont work too hard to evaluate).

(b) What is the magnetization in the high-temperature limit, to lowest non-trivial order (this I want you to evaluate as completely as you can!)?

9.7.28 In a coulomb field

An electron in the Coulomb field of the proton is in the state

$$|\psi\rangle = \frac{4}{5}|1,0,0\rangle + \frac{3i}{5}|2,1,1\rangle$$

where the $|n,\ell,m\rangle$ are the standard energy eigenstates of hydrogen.

(a) What is $\langle E\rangle$ for this state? What are $\left\langle \hat{L}^2 \right\rangle$, $\left\langle \hat{L}_x \right\rangle$ and $\left\langle \hat{L}_x \right\rangle$?

(b) What is $|\psi(t)\rangle$? Which, if any, of the expectation values in (a) vary with time?

9.7.29 Probabilities

(a) Calculate the probability that an electron in the ground state of hydrogen is outside the classically allowed region(defined by the classical turning points)?

(b) An electron is in the ground state of tritium, for which the nucleus is the isotope of hydrogen with one proton and two neutrons. A nuclear reaction instantaneously changes the nucleus into He^3, which consists of two protons and one neutron. Calculate the probability that the electron remains in the ground state of the new atom. Obtain a numerical answer.

9.7.30 What happens?

At the time $t = 0$ the wave function for the hydrogen atom is

$$\psi(\vec{r},0) = \frac{1}{\sqrt{10}}\left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21-1}\right)$$

where the subscripts are the values of the quantum numbers $(n\ell m)$. We ignore spin and any radiative transitions.

(a) What is the expectation value of the energy in this state?

(b) What is the probability of finding the system with $\ell = 1$, $m = +1$ as a function of time?

(c) What is the probability of finding an electron within $10^{-10}\,cm$ of the proton (at time $t = 0$)? A good approximate result is acceptable.

(d) Suppose a measurement is made which shows that $L = 1$, $L_x = +1$. Determine the wave function immediately after such a measurement.

9.7.31 Anisotropic Harmonic Oscillator

In three dimensions, consider a particle of mass m and potential energy

$$V(\vec{r}) = \frac{m\omega^2}{2}\left[(1-\tau)(x^2+y^2) + (1+\tau)z^2\right]$$

where $\omega \geq 0$ and $0 \leq \tau \leq 1$.

(a) What are the eigenstates of the Hamiltonian and the corresponding eigenenergies?

(b) Calculate and discuss, as functions of τ, the variation of the energy and the degree of degeneracy of the ground state and the first two excited states.

9.7.32 Exponential potential

Two particles, each of mass M, are attracted to each other by a potential

$$V(r) = -\left(\frac{g^2}{d}\right)e^{-r/d}$$

where $d = \hbar/mc$ with $mc^2 = 140\,MeV$ and $Mc^2 = 940\,MeV$.

(a) Show that for $\ell = 0$ the radial Schrodinger equation for this system can be reduced to Bessel's differential equation

$$\frac{d^2 J_\rho(x)}{dx^2} + \frac{1}{x}\frac{dJ_\rho(x)}{dx} + \left(1 - \frac{\rho^2}{x^2}\right)J_\rho(x) = 0$$

by means of the change of variable $x = \alpha e^{-\beta r}$ for a suitable choice of α and β.

(b) Suppose that this system is found to have only one bound state with a binding energy of $2.2\,MeV$. Evaluate g^2/d numerically and state its units.

(c) What would the minimum value of g^2/d have to be in order to have two $\ell = 0$ bound state (keep d and M the same). A possibly useful plot is given below in Figure 9.2.

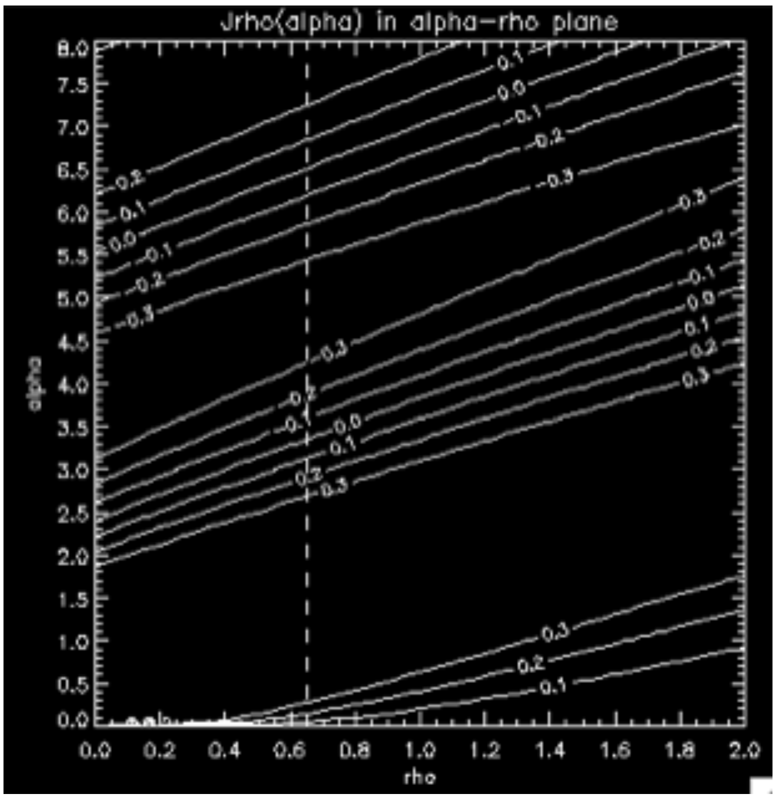

Figure 9.2: $J_\rho(\alpha)$ contours in the $\alpha - \rho$ plane

9.7.33 Bouncing electrons

An electron moves above an impenetrable conducting surface. It is attracted toward this surface by its own image charge so that classically it bounces along the surface as shown in Figure 9.3 below:

(a) Write the Schrodinger equation for the energy eigenstates and the energy eigenvalues of the electron. (Call y the distance above the surface). Ignore inertial effects of the image.

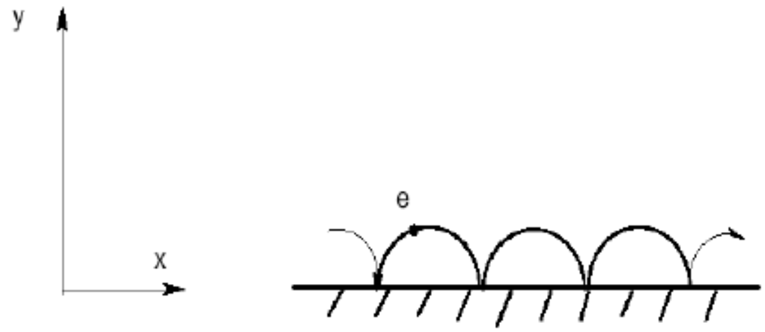

Figure 9.3: Bouncing electrons

(b) What is the x and z dependence of the eigenstates?

(c) What are the remaining boundary conditions?

(d) Find the ground state and its energy? [HINT: they are closely related to those for the usual hydrogen atom]

(e) What is the complete set of discrete and/or continuous energy eigenvalues?

9.7.34 Alkali Atoms

The alkali atoms have an electronic structure which resembles that of hydrogen. In particular, the spectral lines and chemical properties are largely determined by one electron(outside closed shells). A model for the potential in which this electron moves is

$$V(r) = -\frac{e^2}{r}\left(1 + \frac{b}{r}\right)$$

Solve the Schrodinger equation and calculate the energy levels.

9.7.35 Trapped between

A particle of mass m is constrained to move between two concentric impermeable spheres of radii $r = a$ and $r = b$. There is no other potential. Find the ground state energy and the normalized wave function.

9.7.36 Logarithmic potential

A particle of mass m moves in the logarithmic potential

$$V(r) = C\ell n\left(\frac{r}{r_0}\right)$$

Show that:

(a) All the eigenstates have the same mean-squared velocity. Find this mean-squared velocity. Think Virial theorem!

(b) The spacing between any two levels is independent of the mass m.

9.7.37 Spherical well

A spinless particle of mass m is subject (in 3 dimensions) to a spherically symmetric attractive square-well potential of radius r_0.

(a) What is the minimum depth of the potential needed to achieve two bound states of zero angular momentum?

(b) With a potential of this depth, what are the eigenvalues of the Hamiltonian that belong to zero total angular momentum? Solve the transcendental equation where necessary.

9.7.38 In magnetic and electric fields

A point particle of mass m and charge q moves in spatially constant crossed magnetic and electric fields $\vec{B} = B_0\hat{z}$ and $\vec{\mathcal{E}} = \mathcal{E}_0\hat{x}$.

(a) Solve for the complete energy spectrum.

(b) Find the expectation value of the velocity operator

$$\vec{v} = \frac{1}{m}\vec{p}_{mechanical}$$

in the state $\vec{p} = 0$.

9.7.39 Extra(Hidden) Dimensions

Lorentz Invariance with Extra Dimensions

If string theory is correct, we must entertain the possibility that space-time has more than four dimensions. The number of time dimensions must be kept equal to one - it seems very difficult, if not altogether impossible, to construct a consistent theory with more than one time dimension. The extra dimensions must therefore be spatial.

Can we have Lorentz invariance in worlds with more than three spatial dimensions? The answer is yes. Lorentz invariance is a concept that admits a very natural generalization to space-times with additional dimensions.

We first extend the definition of the invariant interval ds^2 to incorporate the additional space dimensions. In a world of five spatial dimensions, for example, we would write

$$ds^2 = c^2dt^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2 - (dx^4)^2 - (dx^5)^2 \tag{9.1}$$

Lorentz transformations are then defined as the linear changes of coordinates that leave ds^2 invariant. This ensures that every inertial observer in the six-dimensional space-time will agree on the value of the speed of light. With more dimensions, come more Lorentz transformations. While in four-dimensional space-time we have boosts in the x^1, x^2 and x^3 directions, in this new world we have boosts along each of the five spatial dimensions. With three spatial coordinates, there are three basic spatial rotations - rotations that mix x^1 and x^2, rotations that mix x^1 and x^3, and finally rotations that mix x^2 and x^3. The equality of the number of boosts and the number of rotations is a special feature of four-dimensional space-time. With five spatial coordinates, we have ten rotations, which is twice the number of boosts.

The higher-dimensional Lorentz invariance includes the lower-dimensional one. If nothing happens along the extra dimensions, then the restrictions of lower-dimensional Lorentz invariance apply. This is clear from equation (9.1). For motion that does not involve the extra dimensions, $dx^4 = dx^5 = 0$, and the expression for ds^2 reduces to that used in four dimensions.

Compact Extra Dimensions

It is possible for additional spatial dimensions to be undetected by low energy experiments if the dimensions are curled up into a compact space of small volume. At this point let us first try to understand what a compact dimension is. We will focus mainly on the case of one dimension. Later we will explain why small compact dimensions are hard to detect.

Consider a one-dimensional world, an infinite line, say, and let x be a coordinate along this line. For each point P along the line, there is a unique real number $x(P)$ called the $x-$coordinate of the point P. A good coordinate on this infinite line satisfies two conditions:

(1) Any two distinct points $P_1 \neq P_2$ have different coordinates $x(P_1) \neq x(P_2)$.

(2) The assignment of coordinates to points are continuous - nearby points have nearly equal coordinates.

If a choice of origin is made for this infinite line, then we can use distance from the origin to define a good coordinate. The coordinate assigned to each point is the distance from that point to the origin, with sign depending upon which side of the origin the point lies.

Imagine you live in a world with one spatial dimension. Suppose you are walking along and notice a strange pattern - the scenery repeats each time you move a distance $2\pi R$ for some value of R. If you meet your friend Phil, you see that there are Phil clones at distances $2\pi R$, $4\pi R$, $6\pi R$, ... down the line as shown in Figure 9.4 below.

In fact, there are clones up the line, as well, with the same spacing.

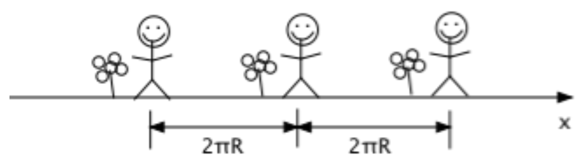

Figure 9.4: Multiple friends

There is no way to distinguish an infinite line with such properties from a circle with circumference $2\pi R$. Indeed, saying that this strange line is a circle *explains* the peculiar property - there really are no Phil clones - you meet the same Phil again and again as you go around the circle!

How do we express this mathematically? We can think of the circle as an open line with an identification, that is, we declare that points with coordinates that differ by $2\pi R$ are the same point. More precisely, two points are declared to be the same point if their coordinates differ by an integer number of $2\pi R$:

$$P_1 \sim P_2 \leftrightarrow x(P_1) = x(P_2) + 2\pi R n \quad , \quad n \in \mathrm{Z} \tag{9.2}$$

This is precise, but somewhat cumbersome, notation. With no risk of confusion, we can simply write

$$x \sim x + 2\pi R \tag{9.3}$$

which should be read as *identify any two points whose coordinates differ by* $2\pi R$. With such an identification, the open line becomes a circle. The identification has turned a non-compact dimension into a compact one. It may seem to you that a line with identifications is only a complicated way to think about a circle. We will se, however, that many physical problems become clearer when we view a compact dimension as an extended one with identifications.

The interval $0 \leq x \leq 2\pi R$ is a *fundamental domain* for the identification (9.3) as shown in Figure 9.5 below.

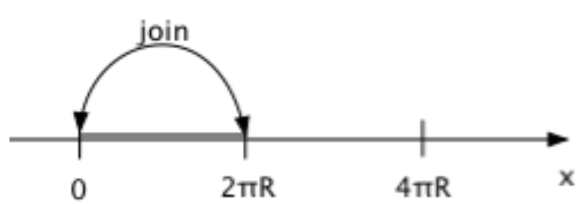

Figure 9.5: Fundamental domain

A fundamental domain is a subset of the entire space that satisfies two conditions:

(1) no two points in are identified

(2) any point in the entire space is related by the identification to some point in the fundamental domain

Whenever possible, as we did here, the fundamental domain is chosen to be a connected region. To build the space implied by the identification, we take the fundamental domain together with its boundary, and implement the identifications on the boundary. In our case, the fundamental domain together with its boundary is the segment $0 \leq x \leq 2\pi R$. In this segment we identify the point $x = 0$ with the point $x = 2\pi R$. The result is the circle.

A circle of radius R can be represented in a two-dimensional plane as the set of points that are a distance R from a point called the center of the circle. Note that the circle obtained above has been constructed directly, without the help of any two-dimensional space. For our circle, there is no point, anywhere, that represents the center of the circle. We can still speak, figuratively, of the radius R of the circle, but in our case, the radius is simply the quantity which multiplied by 2π gives the total length of the circle.

On the circle, the coordinate x is no longer a good coordinate. The coordinate x is now either multi-valued or discontinuous. This is a problem with any coordinate on a circle. Consider using angles to assign coordinates on the unit circle as shown in Figure 9.6 below.

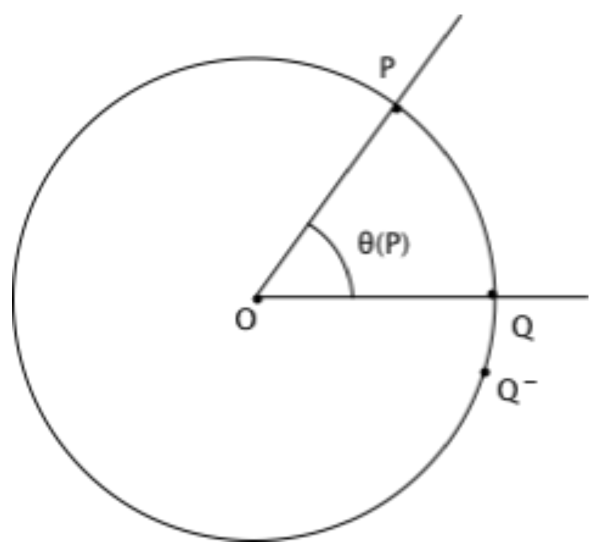

Figure 9.6: Unit circle identification

Fix a reference point Q on the circle, and let O denote the center of the circle. To any point P on the circle we assign as a coordinate the angle $\theta(P) = angle(POQ)$. This angle is naturally multi-valued. The reference point Q, for example, has $\theta(Q) = 0°$ and $\theta(Q) = 360°$. If we force angles to be single-valued by restricting $0° \leq \theta \leq 360°$, for example, then they become discontinuous. Indeed, two nearby points, Q and Q^-, then have very different angles $\theta(Q) = 0°$, while $\theta(Q^-) \sim 360°$. It is easier to work with multi-valued coordinates than it is to work with discontinuous ones.

If we have a world with several open dimensions, then we can apply the identification (9.3) to one of the dimensions, while doing nothing to the others. The dimension described by x turns into a circle, and the other dimensions remain open. It is possible, of course, to make more than one dimension compact.

Consider the example, the (x, y) plane, subject to two identifications,

$$x \sim x + 2\pi R \quad , \quad y \sim y + 2\pi R$$

It is perhaps clearer to show both coordinates simultaneously while writing the identifications. In that fashion, the two identifications are written as

$$(x, y) \sim (x + 2\pi R, y) \quad , \quad (x, y) \sim (x, y + 2\pi R) \tag{9.4}$$

The first identification implies that we can restrict our attention to $0 \leq x \leq 2\pi R$, and the second identification implies that we can restrict our attention to $0 \leq y \leq 2\pi R$. Thus, the fundamental domain can be taken to be the square region $0 \leq x, y < 2\pi R$ as shown in Figure 9.7 below.

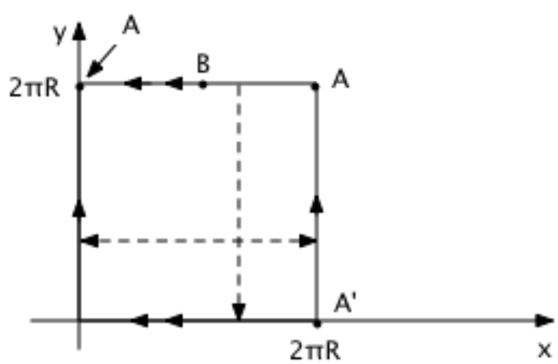

Figure 9.7: Fundamental domain = square

The identifications are indicated by the dashed lines and arrowheads. To build the space implied by the identifications, we take the fundamental domain together with its boundary, forming the full square $0 \leq x, y < 2\pi R$, and implement the identifications on the boundary. The vertical edges are identified because they correspond to points of the form $(0, y)$ and $(2\pi R, y)$, which are identified by the first equation (9.4). This results in the cylinder shown in Figure 9.8 below.

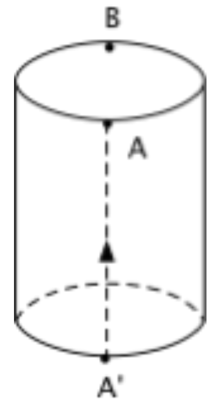

Figure 9.8: Square $\rightarrow$ cylinder

The horizontal edges are identified because they correspond to points of the form $(x, 0)$ and $(x, 2\pi R)$, which are identified by the second equation in (9.4). The resulting space is a two-dimensional torus.

We can visualize this process in Figure 9.9 below.

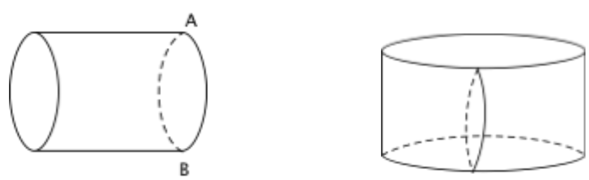

Figure 9.9: 2-dimensional torus

?or in words, the torus is visualized by taking the fundamental domain (with its boundary) and gluing the vertical edges as their identification demands. The result is first (vertical) cylinder shown above (the gluing seam is the dashed line). In this cylinder, however, the bottom circle and the top circle must also be glued, since they are nothing other than the horizontal edges of the fundamental domain. To do this with paper, you must flatten the cylinder and then roll it up and glue the circles. The result looks like a flattened doughnut. With a flexible piece of garden hose, you could simply identify the two ends and obtain the familiar picture of a torus.

We have seen how to compactify coordinates using identifications. Some compact spaces are constructed in other ways. In string theory, however, compact spaces that arise from identifications are particularly easy to work with.

Sometimes identifications have fixed points, points that are related to themselves by the identification. For example, consider the real line parameterized by the coordinate x and subject to the identification $x \sim -x$. The point $x = 0$ is the unique fixed point of the identification. A fundamental domain can be chosen to be the half-line $x \geq 0$. Note that the boundary point $x = 0$ must be included in the fundamental domain. The space obtained by the above identification is in fact the fundamental domain $x \geq 0$. This is the simplest example of an *orbifold*, a space obtained by identifications that have fixed points. This orbifold is called an R^1/Z_2 orbifold. Here R^1 stands for the (one-dimensional) real line, and Z_2 describes a basic property of the identification when it is viewed as the transformation $x \to -x$ - if applied twice, it gives back the original coordinate.

Quantum Mechanics and the Square Well

The fundamental relation governing quantum mechanics is

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

In three spatial dimensions the indices i and j run from 1 to 3. The generalization of quantum mechanics to higher dimensions is straightforward. With d spatial dimensions, the indices simply run over the d possible values.

To set the stage for for the analysis of small extra dimensions, let us review the standard quantum mechanics problem involving and infinite potential well.

The time-independent Schrodinger equation(in one-dimension) is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

In the infinite well system we have

$$V(x) = \begin{cases} 0 & \text{if } x \in (0, a) \\ \infty & \text{if } x \notin (0, a) \end{cases}$$

When $x \in (0, a)$, the Schrodinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

The boundary conditions $\psi(0) = \psi(a) = 0$ give the solutions

$$\psi_k(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{k\pi x}{a}\right) \quad , \quad k = 1, 2, ..., \infty$$

The value $k = 0$ is not allowed since it would make the wave-function vanish everywhere. The corresponding energy values are

$$E_k = \frac{\hbar^2}{2m}\left(\frac{k\pi}{a}\right)^2$$

Square Well with Extra Dimensions

We now add an extra dimension to the square well problem. In addition to x, we include a dimension y that is curled up into a small circle of radius R. In other words, we make the identification

$$(x, y) \sim (x, y + 2\pi R)$$

The original dimension x has not been changed(see Figure 9.10 below). In the figure, on the left we have the original square well potential in one dimension. Here the particle lives on the the line segment shown and on the right, in the (x, y) plane the particle must remain in $0 < x < a$. The direction y is identified as $y \sim y + 2\pi R$.

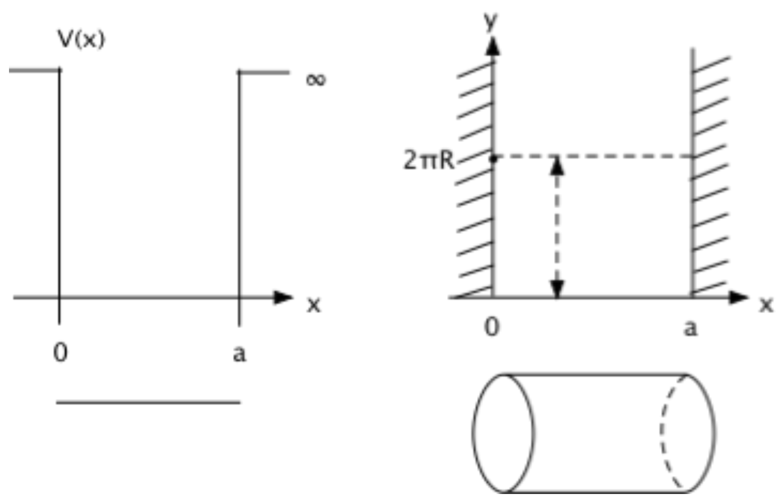

Figure 9.10: Square well with compact hidden dimension

The particle lives on a cylinder, that is, since the y direction has been turned into a circle of circumference $2\pi R$, the space where the particle moves is a cylinder. The cylinder has a length a and a circumference $2\pi R$. The potential energy $V(x,y)$ is given by

$$V(x) = \begin{cases} 0 & \text{if } x \in (0,a) \\ \infty & \text{if } x \notin (0,a) \end{cases}$$

that is, is independent of y.

We want to investigate what happens when R is small and we only do experiments at low energies. Now the only length scale in the one-dimensional infinite well system is the size a of the segment, so small R means $R << a$.

(a) Write down the Schrodinger equation for two Cartesian dimensions.

(b) Use separation of variables to find $x-$dependent and $y-$dependent solutions.

(c) Impose appropriate boundary conditions, namely, and an infinite well in the x dimension and a circle in the y dimension, to determine the allowed values of parameters in the solutions.

(d) Determine the allowed energy eigenvalues and their degeneracy.

(e) Show that the new energy levels contain the old energy levels plus additional levels.

(f) Show that when $R << a$ (a very small (compact) hidden dimension) the first new energy level appears at a very high energy. What are the experimental consequences of this result?

9.7.40 Superfluid Flow

We can discuss macroscopic motions of a superfluid by regarding $\psi(\vec{x},t)$ as a classical wave. We are particularly interested in time-independent and z-independent solutions of the form

$$\psi(x,y) = f(r)e^{in\theta}$$

where $f(r)$ is a real function. Answer the following questions.

(a) Write down the velocity field $\vec{v} = \vec{j}/\rho$ using the number density $\rho = \psi^*\psi$ and the momentum density $\vec{j} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$.

(b) Write down the equation of motion

$$i\hbar\dot{\psi} + \frac{\hbar^2}{2m}\nabla^2\psi + \mu\psi - \lambda\psi^*\psi\psi = 0$$

in terms of $f(r)$. Note that this equation allows a monotonic solution with $f(0) = 0$ and $f(\infty) = \sqrt{\mu/\lambda}$. This solution is called the *vortex solution*.

(c) Show that the velocity field circles around the origin.

(d) Show that the circulation defined by

$$\kappa = \oint \vec{v} \cdot d\vec{l}$$

is quantized.

NOTE: An n-vortex actaully breaks up into n single vortices to lower the energy. Look at the pictures of vortices in regular arrays in rotating superfluid Helium in a paper by E.J. Yarmchuk, M.J.V. Gordon, and R.E Packard, *Observation of Stationary Vortex Arrays in Rotating Superfluid Helium*, Phys. Rev. Lett. **43**, 214-217 (1979).

9.7.41 Spin$-1/2$ Particle in a D-State

A particle of spin$-1/2$ is in a D-state of orbital angular momentum. What are its possible states of total angular momentum? Suppose the single particle Hamiltonian is

$$H = A + B\vec{L} \cdot \vec{S} + C\vec{L} \cdot \vec{L}$$

What are the values of energy for each of the different states of total angular momentum in terms of the constants A, B, and C?

9.7.42 Two Stern-Gerlach Boxes

A beam of spin$-1/2$ particles traveling in the $y-$direction is sent through a Stern-Gerlach apparatus, which is aligned in the $z-$direction, and which divides the incident beam into two beams with $m = \pm 1/2$. The $m = 1/2$ beam is allowed to impinge on a second Stern-Gerlach apparatus aligned along the direction given by

$$\hat{e} = \sin\theta\hat{x} + \cos\theta\hat{z}$$

(a) Evaluate $\vec{S} = (\hbar/2)\,\vec{\sigma} \cdot \hat{e}$, where $\vec{\sigma}$ is represented by the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Calculate the eigenvalues of $\vec{S}$.

(b) Calculate the normalized eigenvectors of $\vec{S}$.

(c) Calculate the intensities of the two beams which emerge from the second Stern-Gerlach apparatus.

9.7.43 A Triple-Slit experiment with Electrons

A beam of spin-1/2 particles are sent into a triple slit experiment according to the figure below.

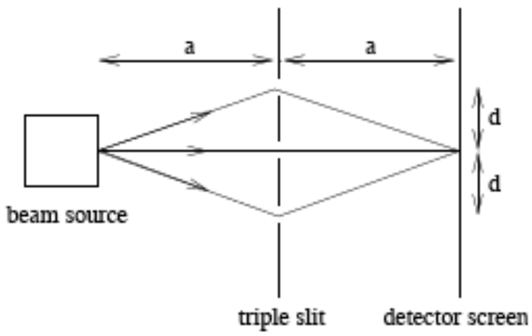

Figure 9.11: Triple-Slit Setup

Calculate the resulting intensity pattern recorded at the detector screen.

9.7.44 Cylindrical potential

The Hamiltonian is given by

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2\mu} + V(\hat{\rho})$$

where $\rho = \sqrt{x^2 + y^2}$.

(a) Use symmetry arguments to establish that both $\hat{p}_z$ and $\hat{L}_z$, the $z-$component of the linear and angular momentum operators, respectively, commute with $\hat{H}$.

(b) Use the fact that $\hat{H}$, $\hat{p}_z$ and $\hat{L}_z$ have eigenstates in common to express the position space eigenfunctions of the Hamiltonian in terms of those of $\hat{p}_z$ and $\hat{L}_z$.

(c) What is the radial equation? Remember that the Laplacian in cylindrical coordinates is

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\varphi^2} + \frac{\partial^2\psi}{\partial z^2}$$

A particle of mass μ is in the cylindrical potential well

$$V(\rho) = \begin{cases} 0 & \rho < a \\ \infty & \rho > a \end{cases}$$

(d) Determine the three lowest energy eigenvalues for states that also have $\hat{p}_z$ and $\hat{L}_z$ equal to zero.

(e) Determine the three lowest energy eigenvalues for states that also have $\hat{p}_z$ equal to zero. The states can have nonzero $\hat{L}_z$.

9.7.45 Crazy potentials.....

(a) A nonrelativistic particle of mass m moves in the potential

$$V(x,y,z) = A(x^2 + y^2 + 2\lambda xy) + B(z^2 + 2\mu z)$$

where $A > 0$, $B > 0$, $|\lambda| < 1$. μ is arbitrary. Find the energy eigenvalues.

(b) Now consider the following modified problem with a new potential

$$V_{new} = \begin{cases} V(x,y,z) & z > -\mu \text{ and any x and y} \\ +\infty & z < -\mu \text{ and any x and y} \end{cases}$$

Find the ground state energy.

9.7.46 Stern-Gerlach Experiment for a Spin-1 Particle

A beam of spin-1 particles, moving along the y-axis, passes through a sequence of two SG devices. The first device has its magnetic field along the $z-$axis and the second device has its magnetic field along the $z'-$axis, which points in the $x-z$ plane at an angle θ relative to the $z-$axis. Both devices only transmit the uppermost beam. What fraction of the particles entering the second device will leave the second device?

9.7.47 Three Spherical Harmonics

As we see, often we need to calculate an integral of the form

$$\int d\Omega Y^*_{\ell_3 m_3}(\theta,\varphi) Y_{\ell_2 m_2}(\theta,\varphi) Y_{\ell_1 m_1}(\theta,\varphi)$$

This can be interpreted as the matrix element $\langle \ell_3 m_3 | \hat{Y}^{(\ell_2)}_{m_2} | \ell_1 m_1 \rangle$, where $\hat{Y}^{(\ell_2)}_{m_2}$ is an irreducible tensor operator.

(a) Use the Wigner-Eckart theorem to determine the restrictions on the quantum numbers so that the integral does not vanish.

(b) Given the *addition rule* for Legendre polynomials:

$$P_{\ell_1}(\mu) P_{\ell_2}(\mu) = \sum_{\ell_3} \langle \ell_3 0 \mid \ell_1 0 \ell_2 0 \rangle^2 P_{\ell_3}(\mu)$$

where $\langle \ell_3 0 \mid \ell_1 0 \ell_2 0\rangle$ is a Clebsch-Gordon coefficient. Use the Wigner-Eckart theorem to prove

$$\begin{aligned}
&\int d\Omega Y^*_{\ell_3 m_3}(\theta,\varphi) Y_{\ell_2 m_2}(\theta,\varphi) Y_{\ell_1 m_1}(\theta,\varphi) \\
&\quad = \sqrt{\frac{(2\ell_2+1)(2\ell_1+1)}{4\pi(2\ell_3+1)}} \langle \ell_3 0 \mid \ell_1 0 \ell_2 0\rangle \langle \ell_3 m_3 \mid \ell_2 m_2 \ell_1 m_1\rangle
\end{aligned}$$

HINT: Consider $\langle \ell_3 0| \hat{Y}_0^{(\ell_2)} |\ell_1 0\rangle$.

9.7.48 Spin operators ala Dirac

Show that

$$\begin{aligned}
\hat{S}_z &= \frac{\hbar}{2} |z+\rangle \langle z+| - \frac{\hbar}{2} |z-\rangle \langle z-| \\
\hat{S}_+ &= \hbar |z+\rangle \langle z-| \quad , \quad \hat{S}_- = \hbar |z-\rangle \langle z+|
\end{aligned}$$

9.7.49 Another spin = 1 system

A particle is known to have spin one. Measurements of the state of the particle yield $\langle S_x\rangle = 0 = \langle S_y\rangle$ and $\langle S_z\rangle = a$ where $0 \le a \le 1$. What is the most general possibility for the state?

9.7.50 Properties of an operator

An operator $\hat{f}$ describing the interaction of two spin$-1/2$ particles has the form $\hat{f} = a + b\vec{\sigma}_1 \cdot \vec{\sigma}_2$ where a and b are constants and $\vec{\sigma}_j = \sigma_{xj}\hat{\mathrm{x}} + \sigma_{yj}\hat{\mathrm{y}} + \sigma_{zj}\hat{\mathrm{z}}$ are Pauli matrix operators. The total spin angular momentum is

$$\vec{j} = \vec{j}_1 + \vec{j}_2 = \frac{\hbar}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)$$

(a) Show that $\hat{f}$, $\vec{j}^2$ and $\hat{j}_z$ can be simultaneously measured.

(b) Derive the matrix representation of $\hat{f}$ in the $|j, m, j_1, j_2\rangle$ basis.

(c) Derive the matrix representation of $\hat{f}$ in the $|j_1, j_2, m_1, m_2\rangle$ basis.

9.7.51 Simple Tensor Operators/Operations

Given the tensor operator form of the particle coordinate operators

$$\vec{r} = (x, y, z);\ R_1^0 = z\ ,\ R_1^{\pm} = \mp\frac{x \pm iy}{\sqrt{2}}$$

(the subscript "1" indicates it is a rank 1 tensor), and the analogously defined particle momentum rank 1 tensor P_1^q, $q = 0, \pm 1$, calculate the commutator between each of the components and show that the results can be written in the form

$$[R_1^q, P_1^m] = \text{ simple expression} \tag{9.5}$$

9.7.52 Rotations and Tensor Operators

Using the rank 1 tensor coordinate operator ? in Problem 9.51, calculate the commutators

$$[L_\pm, R_1^q] \text{ and } [L_z, R_1^q]$$

where $\vec{L}$ is the standard angular momentum operator.

9.7.53 Spin Projection Operators

Show that $\mathcal{P}_1 = \frac{3}{4}\hat{I} + (\vec{S}_1 \cdot \vec{S}_2)/\hbar^2$ and $\mathcal{P}_0 = \frac{1}{4}\hat{I} - (\vec{S}_1 \cdot \vec{S}_2)/\hbar^2$ project onto the spin-1 and spin-0 spaces in $\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$. Start by giving a mathematical statement of just what must be shown.

9.7.54 Two Spins in a magnetic Field

The Hamiltonian of a coupled spin system in a magnetic field is given by

$$H = A + J\frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2} + B\frac{S_{1z} + S_{2z}}{\hbar}$$

where factors of $\hbar$ have been tossed in to make the constants A, J, B have units of energy. [J is called the *exchange constant* and B is proportional to the magnetic field].

(a) Find the eigenvalues and eigenstates of the system when one particle has spin 1 and the other has spin 1/2.

(b) Give the ordering of levels in the low field limit $J \gg B$ and the high field limit $B \gg J$ and interpret physically the result in each case.

9.7.55 Hydrogen d States

Consider the $\ell = 2$ states (for some given principal quantum number n, which is irrelevant) of the H atom, taking into account the electron spin= 1/2 (Neglect nuclear spin!).

(a) Enumerate all states in the J, M representation arising from the $ell = 2$, s= 1/2 states.

(b) Two states have $m_j = M = +1/2$. Identify them and write them precisely in terms of the product space kets $|\ell, m_\ell; s, m_s\rangle$ using the Clebsch-Gordon coefficients.

9.7.56 The Rotation Operator for Spin$-1/2$

We learned that the operator

$$R_n(\Theta) = exp\left(-i\Theta(\vec{e}_n \cdot \hat{\mathbf{J}})/\hbar\right) \tag{9.6}$$

is a *rotation operator*, which rotates a vector about an axis $\vec{e}_n$ by and angle Θ. For the case of spin 1/2,

$$\hat{\mathbf{J}} = \hat{\mathbf{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}} \rightarrow R_n(\Theta) = exp\left(-i\Theta\hat{\sigma}_n/2\right)$$

(a) Show that for spin 1/2

$$R_n(\Theta) = \cos\left(\frac{\Theta}{2}\right)\hat{I} - i\sin\left(\frac{\Theta}{2}\right)\hat{\sigma}_n$$

(b) Show $R_n(\Theta = 2\pi) = -\hat{I}$; Comment.

(c) Consider a series of rotations. Rotate about the $y-$axis by θ followed by a rotation about the $z-$axis by ϕ. Convince yourself that this takes the unit vector along $\vec{e}_z$ to $\vec{e}_n$. Show that up to an overall phase

$$|\uparrow_n\rangle = R_z(\phi)R_y\,|\uparrow_z\rangle$$

9.7.57 The Spin Singlet

Consider the entangled state of two spins

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle_A \otimes |\downarrow_z\rangle_B - |\downarrow_z\rangle_A \otimes |\uparrow_z\rangle_B\right)$$

(a) Show that (up to a phase)

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_n\rangle_A \otimes |\downarrow_n\rangle_B - |\downarrow_n\rangle_A \otimes |\uparrow_n\rangle_B\right)$$

where $|\uparrow_n\rangle$, $|\downarrow_n\rangle$ are spin spin-up and spin-down states along the direction $\vec{e}_n$. Interpret this result.

(b) Show that $\langle\Psi_{AB}|\,\hat{\sigma}_n \otimes \hat{\sigma}_{n'}\,|\Psi_{AB}\rangle = -\vec{e}_n \cdot \vec{e}_{n'}$

9.7.58 A One-Dimensional Hydrogen Atom

Consider the one-dimensional Hydrogen atom, such that the electron confined to the x axis experiences an attractive force e^2/r^2.

(a) Write down Schrodinger's equation for the electron wavefunction $\psi(x)$ and bring it to a convenient form by making the substitutions

$$a = \frac{\hbar^2}{me^2} \quad , \quad E = -\frac{\hbar^2}{2ma^2\alpha^2} \quad , \quad z = \frac{2x}{\alpha a}$$

(b) Solve the Schrodinger equation for $\psi(z)$. (You might need Mathematica, symmetry arguments plus some properties of the Confluent Hypergeometric functions).

(c) Find the three lowest allowed values of energy and the corresponding bound state wavefunctions. Plot them for suitable parameter values.

9.7.59 Electron in Hydrogen $p-$orbital

(a) Show that the solution of the Schrodinger equation for an electron in a p_z-orbital of a hydrogen atom

$$\psi(r,\theta,\phi)=\sqrt{\frac{3}{4\pi}}R_{n\ell}(r)\cos\theta$$

is also an eigenfunction of the square of the angular momentum operator, $\hat{L}^2$, and find the corresponding eigenvalue. Use the fact that

$$\hat{L}^2=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

Given that the general expression for the eigenvalue of $\hat{L}^2$ is $\ell(\ell+1)\hbar^2$, what is the value of the ℓ quantum number for this electron?

(b) In general, for an electron with this ℓ quantum number, what are the allowed values of m_ℓ? (NOTE: you should not restrict yourself to a p_z electron here). What are the allowed values of s and m_s?

(c) Write down the 6 possible pairs of m_s and m_ℓ values for a single electron in a $p-$orbital. Given the Clebsch-Gordon coefficients shown in the table below write down all allowed coupled states $|j,m_j\rangle$ in terms of the

					$\|j,m_j\rangle$		
m_{j_1}	m_{j_2}	$\|3/2,3/2\rangle$	$\|3/2,1/2\rangle$	$\|1/2,1/2\rangle$	$\|3/2,-1/2\rangle$	$\|1/2,-1/2\rangle$	$\|3/2,-3/2\rangle$
1	1/2	1					
1	-1/2		$\sqrt{1/3}$	$\sqrt{2/3}$			
0	1/2		$\sqrt{2/3}$	$-\sqrt{1/3}$			
0	-1/2				$\sqrt{2/3}$	$\sqrt{1/3}$	
-1	1/2				$\sqrt{1/3}$	$-\sqrt{2/3}$	
-1	-1/2						1

Table 9.1: Clebsch-Gordon coefficients for $j_1=1$ and $j_2=1/2$

uncoupled states $|m_\ell,m_s\rangle$. To get started here are the first three:

$$|3/2,3/2\rangle=|1,1/2\rangle$$
$$|3/2,1/2\rangle=\sqrt{2/3}\,|0,1/2\rangle+\sqrt{1/3}\,|1,-1/2\rangle$$
$$|1/2,1/2\rangle=-\sqrt{1/3}\,|0,1/2\rangle+\sqrt{2/3}\,|1,-1/2\rangle$$

(d) The spin-orbit coupling Hamiltonian, $\hat{H}_{so}$ is given by

$$\hat{H}_{so} = \xi(\vec{r})\hat{\ell} \cdot \hat{s}$$

Show that the states with $|j, m_j\rangle$ equal to $|3/2, 3/2\rangle$, $|3/2, 1/2\rangle$ and $|1/2, 1/2\rangle$ are eigenstates of the spin-orbit coupling Hamiltonian and find the corresponding eigenvalues. Comment on which quantum numbers determine the spin-orbit energy. (HINT: there is a rather quick and easy way to do this, so if you are doing something long and tedious you might want to think again .....).

(e) The radial average of the spin-orbit Hamiltonian

$$\int_0^\infty \xi(r)|R_{n\ell}(r)|^2 r^2 dr$$

is called the spin-orbit coupling constant. It is important because it gives the average interaction of an electron in some orbital with its own spin. Given that for hydrogenic atoms

$$\xi(r) = \frac{Ze^2}{8\pi\varepsilon_0 m_e^2 c^2} \frac{1}{r^3}$$

and that for a $2p-$orbital

$$R_{n\ell}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \frac{1}{2\sqrt{6}} \rho e^{-\rho/2}$$

(where $\rho = Zr/a_0$ and $a_0 = 4\pi\varepsilon_0\hbar^2/m_e c^2$) derive an expression for the spin-orbit coupling constant for an electron in a $2p-$orbital. Comment on the dependence on the atomic number Z.

(f) In the presence of a small magnetic field, B, the Hamiltonian changes by a small perturbation given by

$$\hat{H}^{(1)} = \mu_B B(\hat{I}_z + 2\hat{s}_z)$$

The change in energy due to a small perturbation is given in first-order perturbation theory by

$$E^{(1)} = \langle 0| \hat{H}^{(1)} |0\rangle$$

where $|0\rangle$ is the unperturbed state (i.e., in this example, the state in the absence of the applied field). Use this expression to show that the change in the energies of the states in part (d) is described by

$$E^{(1)} = \mu_B B g_j m_j \tag{9.7}$$

and find the values of g_j. We will prove the perturbation theory result in the Chapter 10.

(g) Sketch an energy level diagram as a function of applied magnetic field increasing from $B = 0$ for the case where the spin-orbit interaction is stronger than the electron's interaction with the magnetic field. You can assume that the expressions you derived above for the energy changes of the three states you have been considering are applicable to the other states.

9.7.60 Quadrupole Moment Operators

The quadrupole moment operators can be written as

$$\begin{aligned}
Q^{(+2)} &= \sqrt{\frac{3}{8}}(x+iy)^2 \\
Q^{(+1)} &= -\sqrt{\frac{3}{2}}(x+iy)z \\
Q^{(0)} &= \frac{1}{2}(3z^2-r^2) \\
Q^{(-1)} &= \sqrt{\frac{3}{2}}(x-iy)z \\
Q^{(-2)} &= \sqrt{\frac{3}{8}}(x-iy)^2
\end{aligned}$$

Using the form of the wave function $\psi_{\ell m} = R(r)Y_m^\ell(\theta,\phi)$,

(a) Calculate $\langle\psi_{3,3}|\, Q^{(0)}\, |\psi_{3,3}\rangle$

(b) Predict all others $\langle\psi_{3,m'}|\, Q^{(0)}\, |\psi_{3,m}\rangle$ using the Wigner-Eckart theorem in terms of Clebsch-Gordon coefficients.

(c) Verify them with explicit calculations for $\langle\psi_{3,1}|\, Q^{(0)}\, |\psi_{3,0}\rangle$, $\langle\psi_{3,-1}|\, Q^{(0)}\, |\psi_{3,1}\rangle$ and $\langle\psi_{3,-2}|\, Q^{(0)}\, |\psi_{3,-3}\rangle$.

Note that we leave $\langle r^2\rangle = \int_0^\infty r^2\, dr R^2(r) r^2$ as an overall constant that drops out from the ratios.

9.7.61 More Clebsch-Gordon Practice

Add angular momenta $j_1 = 3/2$ and $j_2 = 1$ and work out all the Clebsch-Gordon coefficients starting from the state $|j,m\rangle = |5/2,5/2\rangle = |3/2,3/2\rangle \otimes |1,1\rangle$.

9.7.62 Spherical Harmonics Properties

(a) Show that L_+ annihilates $Y_2^2 = \sqrt{15/32\pi}\sin^2\theta e^{2i\phi}$.

(b) Work out all of Y_2^m using successive applications of L_- on Y_2^2.

(c) Plot the *shapes* of Y_2^m in 3-dimensions (r,θ,ϕ) using $r = Y_2^m(\theta,\phi)$.

9.7.63 Starting Point for Shell Model of Nuclei

Consider a three-dimensional isotropic harmonic oscillator with Hamiltonian

$$H = \frac{\vec{p}^2}{2m} + \frac{1}{2}m\omega^2\vec{r}^2 = \hbar\omega\left(\vec{a}^+ \cdot \vec{a} + frac32\right)$$

where $\vec{p} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$, $\vec{r} = (\hat{x}_1, \hat{x}_2\hat{x}_2)$, $\vec{a} = (\hat{a}_1, \hat{a}_2, \hat{a}_3)$. We also have the commutators $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$, $[\hat{x}_i, \hat{x}_j] = 0$, $[\hat{p}_i, \hat{p}_j] = 0$, $[\hat{a}_i, \hat{a}_j] = 0$, $[\hat{a}_i^+, \hat{a}_j^+] = 0$, and $[\hat{a}_i, \hat{a}_j^+] = \delta_{ij}$ Answer the following questions.

(a) Clearly, the system is spherically symmetric, and hence there is a conserved angular momentum vector. Show that $\vec{L} = \vec{r} \times \vec{p}$ commutes with the Hamiltonian.

(b) Rewrite $\vec{L}$ in terms of creation and annihilation operators.

(c) Show that $|0\rangle$ belongs to the $\ell = 0$ representation. It is called the $1S$ state.

(d) Show that the operators $\mp(a_1^+ \pm a_2^+)$ and a_3^+ form spherical tensor operators.

(e) Show that $N = 1$ states, $|1,1,\pm 1\rangle = \mp(a_1^+ \pm a_2^+)\,|0\rangle/\sqrt{2}$ and $|1,1,0\rangle = a_3^+\,|0\rangle$, form the $\ell = 1$ representation. (Notation is $|N,\ell,m\rangle$) It is called a $1P$ state because it is the first $P-$state.

(f) Calculate the expectation values of the quadrupole moment $Q = (3z^2 - r^2)$ for $N = \ell = 1$, $m = -1, 0, 1$ states, and verify the Wigner-Eckart theorem.

(g) There are six possible states at the $N = 2$ level. Construct the states $|2,\ell,m\rangle$ with definite $\ell = 0, 2$ and m. They are called $2S$ (because it is second $S-$state) and $1D$ (because it is the first $D-$state).

(h) How many possible states are there at the $N = 3, 4$ levels? What ℓ representations do they fall into?

(i) What can you say about general N?

(j) Verify that the operator $\Pi = e^{i\pi\vec{a}^+\cdot\vec{a}}$ has the correct property as the parity operator by showing that $\Pi\vec{r}\Pi^+ = -\vec{r}$ and $\Pi\vec{p}\Pi^+ = -\vec{p}$.

(k) Show that $\Pi = (-1)^N$

(l) Without calculating it explicitly, show that there are no dipole transitions from the $2P$ state to the $1P$ state. As we will see in Chapter 11, this means, show that $\langle 1P|\,\vec{r}\,|2P\rangle = 0$.

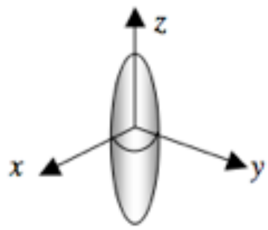

Figure 9.12: Axially Symmetric Rotor

9.7.64 The Axial-Symmetric Rotor

Consider an axially symmetric object which can rotate about any of its axes but is otherwise rigid and fixed. We take the axis of symmetry to be the $z-$axis, as shown below.
The Hamiltonian for this system is

$$\hat{H} = \frac{\hat{L}_x^2 + \hat{L}_y^2}{2I_\perp} + \frac{\hat{L}_z^2}{2I_\parallel}$$

where $I_\perp$ and $I_\parallel$ are the moments of inertia about the principle axes.

(a) Show that the energy eigenvalues and eigenfunctions are respectively

$$E_{\ell,m} = \frac{\hbar^2}{2I_\perp}\left(\ell(\ell+1) - m^2\left(1 - \frac{I_\perp}{I_\parallel}\right)\right) \quad , \quad \psi_{\ell,m} = Y_\ell^m(\theta,\phi)$$

What are the possible values for ℓ and m? What are the degeneracies?

At $t = 0$, the system is prepared in the state

$$\psi_{\ell,m}(t=0) = \sqrt{\frac{3}{4\pi}}\frac{x}{r} = \sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi$$

(b) Show that the state is normalized.

(c) Show that

$$\psi_{\ell,m}(t=0) = \frac{1}{\sqrt{2}}\left(-Y_1^1(\theta,\phi) + Y_1^{-1}(\theta,\phi)\right)$$

(d) From (c) we see that the initial state is *NOT* a single spherical harmonic (the eigenfunctions given in part (a)). Nonetheless, *show* that the wavefunction is an eigenstate of $\hat{H}$ (and thus a stationary state) and find the energy eigenvalue. Explain this.

(e) If one were to measure the observable $\hat{L}^2$ (magnitude of the angular momentum squared) and $\hat{L}_z$, what values could one find and with what probabilities?

9.7.65 Charged Particle in 2-Dimensions

Consider a charged particle on the $x - y$ plane in a constant magnetic field $\vec{B} = (0, 0, B)$ with the Hamiltonian (assume $eB > 0$)

$$H = \frac{\Pi_x^2 + \Pi_y^2}{2m} \quad , \quad \Pi_i = p_i - \frac{e}{c} A_i$$

(a) Use the so-called *symmetric gauge* $\vec{A} = B(-y, x)/2$, and simplify the Hamiltonian using two annihilation operators $\hat{a}_x$ and $\hat{a}_y$ for a suitable choice of ω.

(b) Further define $\hat{a}_z = (\hat{a}_x + i\hat{a}_y)/2$ and $\hat{a}_{\bar{z}} = (\hat{a}_x - i\hat{a}_y)/2$ and then rewrite the Hamiltonian using them. General states are given in the form

$$|n, m\rangle = \frac{(\hat{a}_z^+)^n}{\sqrt{n!}} \frac{\left(\hat{a}_{\bar{z}}^+\right)^m}{\sqrt{m!}} |0, 0\rangle$$

starting from the ground state where $\hat{a}_z |0, 0\rangle = \hat{a}_{\bar{z}} |0, 0\rangle = 0$. Show that they are Hamiltonian eigenstates of energies $\hbar\omega(2n + 1)$.

(c) For an electron, what is the excitation energy when $B = 100\, kG$?

(d) Work out the wave function $\langle x, y \,|\, 0, 0\rangle$ in position space.

(e) $|0, m\rangle$ are all ground states. Show that their position-space wave functions are given by

$$\psi_{0,m}(z, \bar{z}) = N z^m e^{-eB\bar{z}z/4\hbar c}$$

where $z = x + iy$ and $\bar{z} = x - iy$. Determine N.

(f) Plot the probability density of the wave function for $m = 0, 3, 10$ on the same scale (use ContourPlot or Plot3D in Mathematica).

(g) Assuming that the system is a circle of finite radius R, show that there are only a finite number of ground states. Work out the number approximately for large R.

(h) Show that the coherent state $e^{f\hat{a}_z^+} |0, 0\rangle$ represents a near-classical cyclotron motion in position space.

9.7.66 Particle on a Circle Again

A particle of mass m is allowed to move only along a circle of radius R on a plane, $x = R\cos\theta$, $y = R\sin\theta$.

(a) Show that the Lagrangian is $L = mR^2\dot{\theta}^2/2$ and write down the canonical momentum p_θ and the Hamiltonian.

(b) Write down the Heisenberg equations of motion and solve them, (So far no representation was taken).

(c) Write down the normalized position-space wave function $\psi_k(\theta) = \langle \theta \mid k \rangle$ for the momentum eigenstates $\hat{p}_\theta \left| k \right\rangle = \hbar k \left| k \right\rangle$ and show that only $k = n \in \mathbb{Z}$ are allowed because of the requirement $\psi(\theta + 2\pi) = \psi(\theta)$.

(d) Show the orthonormality

$$\langle n \mid m \rangle = \int_0^{2\pi} \psi_n^* \psi_m \, d\theta = \delta_{nm}$$

(e) Now we introduce a constant magnetic field B inside the radius $r < d < R$ but no magnetic field outside $r > d$. Prove that the vector potential is

$$(A_x, A_y) = \begin{cases} B(-y, x)/2 & r < d \\ Bd^2(-y, x)/2r^2 & r > d \end{cases} \tag{9.8}$$

Write the Lagrangian, derive the Hamiltonian and show that the energy eigenvalues are influenced by the magnetic field even though the particle does not *see* the magnetic field directly.

9.7.67 Density Operators Redux

(a) Find a valid density operator ρ for a spin$-1/2$ system such that

$$\langle S_x \rangle = \langle S_y \rangle = \langle S_z \rangle = 0$$

Remember that for a state represented by a density operator ρ we have $\langle O_q \rangle = Tr[\rho O_q]$. Your density operator should be a 2×2 matrix with trace equal to one and eigenvalues $0 \leq \lambda \leq 1$. Prove that ρ you find does not correspond to a pure state and therefore cannot be represented by a state vector.

(b) Suppose that we perform a measurement of the projection operator P_i and obtain a positive result. The projection postulate (reduction postulate) for pure states says

$$\left| \Psi \right\rangle \mapsto \left| \Psi \right\rangle_i = \frac{P_i \left| \Psi \right\rangle}{\sqrt{\left\langle \Psi \right| P_i \left| \Psi \right\rangle}}$$

Use this result to show that in density operator notation $\rho = \left| \Psi \right\rangle \left\langle \Psi \right|$ maps to

$$\rho_i = \frac{P_i \rho P_i}{Tr[\rho P_i]}$$

9.7.68 Angular Momentum Redux

(a) Define the angular momentum operators L_x, L_y, L_z in terms of the position and momentum operators. Prove the following commutation result for these operators: $[L_x, L_y] - i\hbar L_z$.

(b) Show that the operators $L_\pm = L_x \pm iL_y$ act as raising and lowering operators for the z component of angular momentum by first calculating the commutator $[L_z, L_\pm]$.

(c) A system is in state ψ, which is an eigenstate of the operators L^2 and L_z with quantum numbers ell and m. Calculate the expectation values $\langle L_x \rangle$ and $\langle L_x^2 \rangle$. HINT: express L_x in terms of $L_\pm$.

(d) Hence show that L_x and L_y satisfy a general form of the uncertainty principle:

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq -\frac{1}{4} \langle [A, B] \rangle$$

9.7.69 Wave Function Normalizability

The time-independent Schrodinger equation for a spherically symmetric potential $V(r)$ is

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) - \frac{\ell(\ell+1)}{r^2} \right] = (E - V)R$$

where $\psi = R(r) Y_\ell^m(\theta, \phi)$, so that the particle is in an eigenstate of angular momentum.

Suppose $R(r) \propto r^{-\alpha}$ and $V(r) \propto -r^{-\beta}$ near the origin. Show that $\alpha < 3/2$ is required if the wavefunction is to be normalizable, but that $\alpha < 1/2$ (or $\alpha < (3 - \beta)/2$ if $\beta > 2$) is required for the expectation value of energy to be finite.

9.7.70 Currents

The quantum flux density of probability is

$$\vec{j} = \frac{i\hbar}{2m} \left(\psi \nabla \psi^* - \psi^* \nabla \psi \right)$$

It is related to the probability density $\rho = |\psi|^2$ by $\nabla \cdot \vec{j} + \dot{\rho} = 0$.

(a) Consider the case where ψ is a stationary state. Show thet ρ and $\vec{j}$ are then independent of time/ Show that, in one spatial dimension, $\vec{j}$ is also independent of position.

(b) Consider a 3D plane wave $\psi = Aexp(i\vec{k} \cdot \vec{x})$. What is $\vec{j}$ in this case? Give a physical interpretation.

9.7.71 Pauli Matrices and the Bloch Vector

(a) Show that the Pauli operators

$$\sigma_x = \frac{2}{\hbar} S_x \quad , \quad \sigma_y = \frac{2}{\hbar} S_y \quad , \quad \sigma_z = \frac{2}{\hbar} S_z$$

satisfy

$$Tr[\sigma_i, \sigma j] = 2\delta_{ij}$$

where the indices i and j can take on the values x, y or z. You will probably want to work with matrix representations of the operators.

(b) Show that the Bloch vectors for a spin$-1/2$ degree of freedom

$$\vec{s} = \langle S_x \rangle \hat{x} + \langle S_y \rangle \hat{y} + \langle S_z \rangle \hat{z}$$

has length$\hbar/2$ if and only if the corresponding density operator represents a pure state. You may wish to make use of the fact that an arbitrary spin$-1/2$ density operator can be parameterized in the following way:

$$\rho = \frac{1}{2} \left(I + \langle \sigma_x \rangle \sigma_x + \langle \sigma_y \rangle \sigma_y + \langle \sigma_z \rangle \sigma_z \right)$$

Chapter 10

Time-Independent Perturbation Theory

10.9 Problems

10.9.1 Box with a *Sagging Bottom*

Consider a particle in a 1−dimensional box with a *sagging bottom* given by

$$V(x) = \begin{cases} -V_0 sin(\pi x/L) & \text{for } 0 \leq x \leq L \\ \infty & \text{for } x < 0 \text{ and } x > L \end{cases}$$

(a) For small V_0 this potential can be considered as a small perturbation of an infinite box with a flat bottom, for which we have already solved the Schrodinger equation. What is the perturbation potential?

(b) Calculate the energy shift due to the sagging for the particle in the n^{th} stationary state to first order in the perturbation.

10.9.2 Perturbing the Infinite Square Well

Calculate the first order energy shift for the first three states of the infinite square well in one dimension due to the perturbation

$$V(x) = V_0 \frac{x}{a}$$

as shown in Figure 10.1 below.

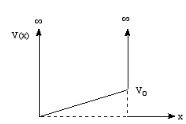

Figure 10.1: Ramp perturbation

10.9.3 Weird Perturbation of an Oscillator

A particle of mass m moves in one dimension subject to a harmonic oscillator potential $\frac{1}{2}m\omega^2 x^2$. The particle is perturbed by an additional weak anharmonic force described by the potential $\Delta V = \lambda \sin kx$, $\lambda << 1$. Find the corrected ground state.

10.9.4 Perturbing the Infinite Square Well Again

A particle of mass m moves in a one dimensional potential box

$$V(x) = \begin{cases} \infty & \text{for } |x| > 3a \\ 0 & \text{for } a < x < 3a \\ 0 & \text{for } -3a < x < -a \\ V_0 & \text{for } |x| < a \end{cases}$$

as shown in Figure 10.2 below.

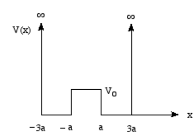

Figure 10.2: Square bump perturbation

Use first order perturbation theory to calculate the new energy of the ground state.

10.9.5 Perturbing the 2-dimensional Infinite Square Well

Consider a particle in a 2-dimensional infinite square well given by

$$V(x,y) = \begin{cases} 0 & \text{for } 0 \le x \le a \text{ and } 0 \le y \le a \\ \infty & \text{otherwise} \end{cases}$$

(a) What are the energy eigenvalues and eigenkets for the three lowest levels?

(b) We now add a perturbation given by

$$V_1(x,y) = \begin{cases} \lambda xy & \text{for } 0 \le x \le a \text{ and } 0 \le y \le a \\ 0 & \text{otherwise} \end{cases}$$

Determine the first order energy shifts for the three lowest levels for $\lambda \ll 1$.

(c) Draw an energy diagram with and without the perturbation for the three energy states, Make sure to specify which unperturbed state is connected to which perturbed state.

10.9.6 Not So Simple Pendulum

A mass m is attached by a massless rod of length L to a pivot P and swings in a vertical plane under the influence of gravity as shown in Figure 10.3 below.

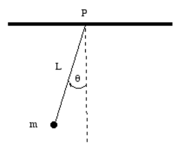

Figure 10.3: A quantum pendulum

(a) In the small angle approximation find the quantum mechanical energy levels of the system.

(b) Find the lowest order correction to the ground state energy resulting from the inaccuracy of the small angle approximation.

10.9.7 1-Dimensional Anharmonic Oscillator

Consider a particle of mass m in a $1-$dimensional anharmonic oscillator potential with potential energy

$$V(x) = \frac{1}{2}m\omega^2 x^2 + \alpha x^3 + \beta x^4$$

(a) Calculate the $1^{st}-$order correction to the energy of the n^{th} perturbed state. Write down the energy correct to $1^{st}-$order.

(b) Evaluate all the required matrix elements of x^3 and x^4 needed to determine the perturbed energy levels and the wave function of the n^{th} state perturbed to $1^{st}-$order.

10.9.8 A Relativistic Correction for Harmonic Oscillator

A particle of mass m moves in a $1-$dimensional oscillator potential

$$V(x) = \frac{1}{2}m\omega^2 x^2$$

In the nonrelativistic limit, where the kinetic energy and the momentum are related by

$$T = \frac{p^2}{2m}$$

the ground state energy is well known to be $E_0 = \hbar\omega/2$.

Relativistically, the kinetic energy and the momentum are related by

$$T = E - mc^2 = \sqrt{m^2c^4 + p^2c^2} - mc^2$$

(a) Determine the lowest order correction to the kinetic energy (a p^4 term).

(b) Consider the correction to the kinetic energy as a perturbation and compute the relativistic correction to the ground state energy.

10.9.9 Degenerate perturbation theory on a spin $= 1$ system

Consider the spin Hamiltonian for a system of spin $= 1$

$$\hat{H} = A\hat{S}_z^2 + B(\hat{S}_x^2 - \hat{S}_y^2) \quad , \quad B << A$$

This corresponds to a spin $= 1$ ion located in a crystal with rhombic symmetry.

(a) Solve the unperturbed problem for $\hat{H}_0 = A\hat{S}_z^2$.

(b) Find the perturbed energy levels to first order.

(c) Solve the problem exactly by diagonalizing the Hamiltonian matrix in some basis. Compare to perturbation results.

10.9.10 Perturbation Theory in Two-Dimensional Hilbert Space

Consider a spin$-1/2$ particle in the presence of a static magnetic field along the z and x directions,

$$\vec{B} = B_z\hat{e}_z + B_x\hat{e}_x$$

(a) Show that the Hamiltonian is

$$\hat{H} = \hbar\omega_0\hat{\sigma}_z + \frac{\hbar\Omega}{2}\hat{\sigma}_x$$

where $\hbar\omega_0 = \mu_B B_z$ and $\hbar\Omega_0 = 2\mu_B B_x$.

(b) If $B_x = 0$, the eigenvectors are $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$ with eigenvalues $\pm\hbar\omega_0$respectively. Now turn on a weak x field with $B_x \ll B_z$. Use perturbation theory to find the new eigenvectors and eigenvalues to lowest order in B_x/B_z.

(c) Suppose now $B_z = 0$. What are the eigenvectors and eigenvalues in terms of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$. Relate this result to degenerate perturbation theory.

(d) This problem can actually be solved exactly. Find the eigenvectors and eigenvalues for arbitrary values of B_z and B_x. Show that these agree with your results in parts (b) and (c) by taking appropriate limits.

(e) Plot the energy eigenvalues as a function of B_z for fixed B_x. Label the eigenvectors on the curves when $B_z = 0$ and when $B_z \to \pm\infty$.

10.9.11 Finite Spatial Extent of the Nucleus

In most discussions of atoms, the nucleus is treated as a positively charged point particle. In fact, the nucleus does possess a finite size with a radius given approximately by the empirical formula

$$R \approx r_0 A^{1/3}$$

where $r_0 = 1.2 \times 10^{-13}\,cm$ (i.e., 1.2 Fermi) and A is the atomic weight or number (essentially the number of protons and neutrons in the nucleus). A reasonable assumption is to take the total nuclear charge $+Ze$ as being uniformly distributed over the entire nuclear volume (assumed to be a sphere).

(a) Derive the following expression for the electrostatic potential energy of an electron in the field of the *finite* nucleus:

$$V(r) = \begin{cases} -\frac{Ze^2}{r} & \text{for } r > R \\ \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2}\right) & \text{for } r < R \end{cases}$$

Draw a graph comparing this potential energy and the point nucleus potential energy.

(b) Since you know the solution of the point nucleus problem, choose this as the unperturbed Hamiltonian $\hat{H}_0$ and construct a perturbation Hamiltonian $\hat{H}_1$ such that the total Hamiltonian contains the $V(r)$ derived above. Write an expression for $\hat{H}_1$.

(c) Calculate(remember that $R \ll a_0 =$ Bohr radius) the $1^{st}-$order perturbed energy for the $1s$ $(n\ell m) = (100)$ state obtaining an expression in terms of Z and fundamental constants. How big is this result compared to the ground state energy of hydrogen? How does it compare to hyperfine splitting?

10.9.12 Spin-Oscillator Coupling

Consider a Hamiltonian describing a spin$-1/2$ particle in a harmonic well as given below:

$$\hat{H}_0 = \frac{\hbar\omega}{2}\hat{\sigma}_z + \hbar\omega\left(\hat{a}^+\hat{a} + 1/2)\right)$$

(a) Show that

$$\{|n\rangle \otimes |\downarrow\rangle = |n,\downarrow\rangle \ , \ |n\rangle \otimes |\uparrow\rangle = |n,\uparrow\rangle\}$$

are energy eigenstates with eigenvalues $E_{n,\downarrow} = n\hbar\omega$ and $E_{n,\uparrow} = (n+1)\hbar\omega$, respectively.

(b) The states associated with the ground-state energy and the first excited energy level are

$$\{|0,\downarrow\rangle \ , \ |1,\downarrow\rangle \ , \ |0,\uparrow\rangle\}$$

What is(are) the ground state(s)? What is(are) the first excited state(s)? Note: two states are degenerate.

(c) Now consider adding an interaction between the harmonic motion and the spin, described by the Hamiltonian

$$\hat{H}_1 = \frac{\hbar\Omega}{2}\left(\hat{a}\hat{\sigma}_+ + \hat{a}^+\hat{\sigma}_-\right)$$

so that the total Hamiltonian is now $\hat{H} = \hat{H}_0 + \hat{H}_1$. Write a matrix representation of $\hat{H}$ in the subspace of the ground and first excited states in the ordered basis given in part (b).

(d) Find the first order correction to the ground state and excited state energy eigenvalues for the subspace above.

10.9.13 Motion in spin-dependent traps

Consider an electron moving in one dimension, in a spin-dependent trap as shown in Figure 10.4 below:

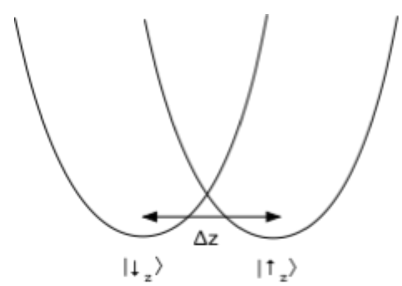

Figure 10.4: A spin-dependent trap

If the electron is in a spin-up state (with respect to the $z-$axis), it is trapped in the right harmonic oscillator well and if it is in a spin-down state (with respect to the $z-$axis), it is trapped in the left harmonic oscillator well. The Hamiltonian that governs its dynamics can be written as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_{osc}^2(\hat{z} - \Delta z/2)^2 \otimes |\uparrow_z\rangle\langle\uparrow_z| + \frac{1}{2}m\omega_{osc}^2(\hat{z} + \Delta z/2)^2 \otimes |\downarrow_z\rangle\langle\downarrow_z|$$

(a) What are the energy levels and stationary states of the system? What are the degeneracies of these states? Sketch an energy level diagram for the first three levels and label the degeneracies.

(b) A small, constant *transverse field* B_x is now added with $|\mu_B B_x| << \hbar\omega_{osc}$. Qualitatively sketch how the energy plot in part (a) is modified.

(c) Now calculate the perturbed energy levels for this system.

(d) What are the new eigenstates in the ground-state doublet? For Δz macroscopic, these are sometimes called Schrodinger cat states. Explain why.

10.9.14 Perturbed Oscillator

A particle of mass m is moving in the 3−dimensional harmonic oscillator potential

$$V(x,y,z) = \frac{1}{2}m\omega^2(x^2+y^2+z^2)$$

A weak perturbation is applied in the form of the function

$$\Delta V(x,y,z) = kxyz + \frac{k^2}{\hbar\omega}x^2y^2z^2$$

where k is a small constant. Calculate the shift in the ground state energy to *second order* in k. This is *not the same* as second-order perturbation theory!

10.9.15 Another Perturbed Oscillator

Consider the system described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2\alpha}(1-e^{-\alpha x^2})$$

Assume that $\alpha << m\omega/\hbar$

(1) Calculate an approximate value for the ground state energy using first-order perturbation theory by perturbing the harmonic oscillator Hamiltonian

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

(2) Calculate an approximate value for the ground state energy using the variational method with a trial function $\psi = e^{-\beta x^2/2}$.

10.9.16 Helium from Hydrogen - 2 Methods

(a) Using a simple hydrogenic wave function for each electron, calculate by perturbation theory the energy in the ground state of the He atom associated with the electron-electron Coulomb interaction. Use this result to estimate the ionization energy of Helium.

(b) Calculate the ionization energy by using the variational method with an effective charge λ in the hydrogenic wave function as the variational parameter.

(c) Compare (a) and (b) with the experimental ionization energy

$$E_{ion} = 1.807E_0 \quad , \quad E_0 = \frac{\alpha^2 mc^2}{2} \quad , \quad \alpha = \text{ fine structure constant}$$

You will need

$$\psi_{1s}(r) = \sqrt{\frac{\lambda^3}{\pi}}\exp(-\lambda r) \quad , \quad a_0 = \frac{\hbar^2}{me^2} \quad , \quad \int\int d^3r_1 d^3r_2 \frac{e^{-\beta(r_1+r_2)}}{|\vec{r}_1-\vec{r}_2|} = \frac{20\pi^2}{\beta^5}$$

That last integral is very hard to evaluate from first principles.

10.9.17 Hydrogen atom + xy perturbation

An electron moves in a Coulomb field centered at the origin of coordinates. The first excited state ($n = 2$) is $4-$fold degenerate. Consider what happens in the presence of a non-central perturbation

$$V_{pert} = f(r)xy$$

where $f(r)$ is some function only of r, which falls off rapidly as $r \to \infty$. To first order, this perturbation splits the $4-$fold degenerate level into several distinct levels (some might still be degenerate).

(a) How many levels are there?

(b) What is the degeneracy of each?

(c) Given the energy shift, call it ΔE, for one of the levels, what are the values of the shifts for all the others?

10.9.18 Rigid rotator in a magnetic field

Suppose that the Hamiltonian of a rigid rotator in a magnetic field is of the form

$$\hat{H} = A\vec{L}^2 + B\hat{L}_z + C\hat{L}_y$$

Assuming that $A\,,\,B \gg C$, use perturbation theory to lowest nonvanishing order to get approximate energy eigenvalues.

10.9.19 Another rigid rotator in an electric field

Consider a rigid body with moment of inertia I, which is constrained to rotate in the $xy-$plane, and whose Hamiltonian is

$$\hat{H} = \frac{1}{2I}\hat{L}_z^2$$

Find the eigenfunctions and eigenvalues (zeroth order solution). Now assume the rotator has a fixed dipole moment $\vec{p}$ in the plane. An electric field $\vec{\mathcal{E}}$ is applied in the plane. Find the change in the energy levels to first and second order in the field.

10.9.20 A Perturbation with 2 Spins

Let $\vec{S}_1$ and $\vec{S}_2$ be the spin operators of two spin$-1/2$ particles. Then $\vec{S} = \vec{S}_1 + \vec{S}_2$ is the spin operator for this two-particle system.

(a) Consider the Hamiltonian

$$\hat{H}_0 = \alpha(\hat{S}_x^2 + \hat{S}_y^2 - \hat{S}_z^2)/\hbar^2$$

Determine its eigenvalues and eigenvectors.

(b) Consider the perturbation $\hat{H}_1 = \lambda(\hat{S}_{1x} - \hat{S}_{2x})$. Calculate the new energies in first-order perturbation theory.

10.9.21 Another Perturbation with 2 Spins

Consider a system with the unperturbed Hamiltonian $\hat{H}_0 = -A(\hat{S}_{1z} + \hat{S}_{2z})$ with a perturbing Hamiltonian of the form $\hat{H}_1 = B(\hat{S}_{1x}\hat{S}_{2x} - \hat{S}_{1y}\hat{S}_{2y})$.

(a) Calculate the eigenvalues and eigenvectors of ?$\hat{H}_0$

(b) Calculate the exact eigenvalues of $\hat{H}_0 + \hat{H}_1$

(c) By means of perturbation theory, calculate the first- and the second-order shifts of the ground state energy of $\hat{H}_0$, as a consequence of the perturbation $\hat{H}_1$. Compare these results with those of (d).

10.9.22 Spherical cavity with electric and magnetic fields

Consider a spinless particle of mass m and charge e confined in spherical cavity of radius R, that is, the potential energy is zero for $r < R$ and infinite for $r > R$.

(a) What is the ground state energy of this system?

(b) Suppose that a weak uniform magnetic field of strength B is switched on. Calculate the shift in the ground state energy.

(c) Suppose that, instead a weak uniform electric field of strength $\mathcal{E}$ is switched on. Will the ground state energy increase or decrease? Write down, but do not attempt to evaluate, a formula for the shift in the ground state energy due to the electric field.

(d) If, instead, a very strong magnetic field of strength B is turned on, approximately what would be the ground state energy?

10.9.23 Hydrogen in electric and magnetic fields

Consider the $n = 2$ levels of a hydrogen-like atom. Neglect spins. Calculate to lowest order the energy splittings in the presence of both electric and magnetic fields $\vec{B} = B\hat{e}_z$ and $\vec{\mathcal{E}} = \mathcal{E}\hat{e}_x$.

10.9.24 $n = 3$ Stark effect in Hydrogen

Work out the Stark effect to lowest nonvanishing order for the $n = 3$ level of the hydrogen atom. Obtain the energy shifts and the zeroth order eigenkets.

10.9.25 Perturbation of the $n = 3$ level in Hydrogen - Spin-Orbit and Magnetic Field corrections

In this problem we want to calculate the 1st-order correction to the n=3 unperturbed energy of the hydrogen atom due to spin-orbit interaction and magnetic field interaction for arbitrary strength of the magnetic field. We have

$\hat{H} = \hat{H}_0 + \hat{H}_{so} + \hat{H}_m$ where

$$\hat{H}_0 = \frac{\vec{p}_{op}^{\,2}}{2m} + V(r) \quad , \quad V(r) = -e^2\left(\frac{1}{r}\right)$$
$$\hat{H}_{so} = \left[\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right]\vec{S}_{op}\cdot\vec{L}_{op}$$
$$\hat{H}_m = \frac{\mu_B}{\hbar}(\vec{L}_{op} + 2\vec{S}_{op})\cdot\vec{B}$$

We have two possible choices for basis functions, namely,

$$|n\ell s m_\ell m_s\rangle \quad or \quad |n\ell s j m_j\rangle$$

The former are easy to write down as direct-product states

$$|n\ell s m_\ell m_s\rangle = R_{n\ell}(r)Y_\ell^{m_\ell}(\theta,\varphi)\,|s, m_s\rangle$$

while the latter must be constructed from these direct-product states using addition of angular momentum methods. The perturbation matrix is not diagonal in either basis. The number of basis states is given by

$$\sum_{\ell=0}^{n-1=2}(2\ell+1)\times 2 = 10 + 6 + 2 = 18$$

All the 18 states are degenerate in zero-order. This means that we deal with an 18×18 matrix (mostly zeroes) in degenerate perturbation theory.

Using the direct-product states

(a) Calculate the nonzero matrix elements of the perturbation and arrange them in block-diagonal form.

(b) Diagonalize the blocks and determine the eigenvalues as functions of B.

(c) Look at the $B \to 0$ limit. Identify the spin-orbit levels. Characterize them by $(\ell s j)$.

(d) Look at the large B limit. Identify the Paschen-Bach levels.

(e) For small B show the Zeeman splittings and identify the Lande $g-$factors.

(f) Plot the eigenvalues versus B.

10.9.26 Stark Shift in Hydrogen with Fine Structure

Excluding nuclear spin, the $n = 2$ spectrum of Hydrogen has the configuration:

where $\Delta E_{FS}/\hbar = 10\ GHz$ (the fine structure splitting) and $\Delta E_{Lamb}/\hbar = 1\ GHz$ (the Lamb shift - an effect of quantum fluctuations of the electromagnetic field). These shifts were neglected in the text discussion of the Stark effect. This is valid if $ea_0E_z >> \Delta E$. Let $x = ea_0E_z$.

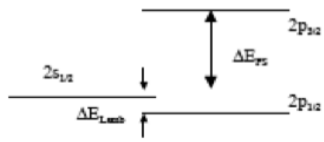

Figure 10.5: $n = 2$ Spectrum in Hydrogen

(a) Suppose $x < \Delta E_{Lamb}$, but $x << \Delta E_{FS}$. . Then we need only consider the $(2s_{1/2}, 2p_{1/2})$ subspace in a near degenerate case. Find the new energy eigenvectors and eigenvalues to first order. Are they degenerate? For what value of the field (in volts/cm) is the level separation doubled over the zero field Lamb shift? HINT: Use the representation of the fine structure eigenstates in the uncoupled representation.

(b) Now suppose $x > \Delta E_{FS}$. We must include all states in the near degenerate case. Calculate and plot numerically the eigenvalues as a function of x, in the range from $0\,GHz < x < 10\,GHz$.

Comment on the behavior of these curves. Do they have the expected asymptotic behavior? Find analytically the eigenvectors in the limit $x/\Delta E_{FS} \to \infty$. Show that these are the expected perturbed states.

10.9.27 2-Particle Ground State Energy

Estimate the ground state energy of a system of two interacting particles of mass m_1 and m_2 with the interaction energy

$$U(\vec{r}_1 - \vec{r}_2) = C\left(|\vec{r}_1 - \vec{r}_2|^4\right)$$

using the variational method.

10.9.28 1s2s Helium Energies

Use first-order perturbation theory to estimate the energy difference between the singlet and triple states of the (1s2s) configuration of helium. The 2s single particle state in helium is

$$\psi_{2s}(\vec{r}) = \frac{1}{\sqrt{4\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2 - \frac{2r}{a_0}\right)e^{-r/a_0}$$

10.9.29 Hyperfine Interaction in the Hydrogen Atom

Consider the interaction

$$H_{hf} = \frac{\mu_B \mu_N}{a_B^3}\frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2}$$

where μ_B , μ_N are the Bohr magneton and the nuclear magneton, a_B is the Bohr radius, and $\vec{S}_1$, $\vec{S}_2$ are the proton and electron spin operators.

(a) Show that H_{hf} splits the ground state into two levels:

$$E_t = -1\ Ry + \frac{A}{4} \quad , \quad E_s = -1\ Ry - \frac{3A}{4}$$

and that the corresponding states are triplets and singlets, respectively.

(b) Look up the constants, and obtain the frequency and wavelength of the radiation that is emitted or absorbed as the atom jumps between the states. The use of hyperfine splitting is a common way to detect hydrogen, particularly intergalactic hydrogen.

10.9.30 Dipole Matrix Elements

Complete with care; this is real physics. The charge dipole operator for the electron in a hydrogen atom is given by

$$\vec{d}(\vec{r}) = -e\vec{r}$$

Its expectation value in any state vanishes (you should be able to see why easily), but its matrix elements between different states are important for many applications (transition amplitudes especially).

(a) Calculate the matrix elements of each of the components between the 1s ground state and each of the 2p states(there are three of them). By making use of the Wigner-Eckart theorem (which you naturally do without thinking when doing the integral) the various quantities are reduced to a single *irreducible* matrix element and a very manageable set of Clebsch-Gordon coefficients.

(b) By using actual H-atom wavefunctions (normalized) obtain the magnitude of quantities as well as the angular dependence (which at certain points at least are encoded in terms of the (ℓ, m) indices).

(c) Reconstruct the vector matrix elements

$$\langle 1s|\, \vec{d}\, |2p_j\rangle$$

and discuss the angular dependence you find.

10.9.31 Variational Method 1

Let us consider the following very simple problem to see how good the variational method works.

(a) Consider the 1−dimensional harmonic oscillator. Use a Gaussian trial wave function $\psi_n(x) = e^{-\alpha x^2}$. Show that the variational approach gives the exact ground state energy.

(b) Suppose for the trial function, we took a Lorentzian

$$\psi_n(x) = \frac{1}{x^2 + \alpha}$$

Using the variational method, by what percentage are you off from the exact ground state energy?

(c) Now consider the *double oscillator* with potential

$$V(x) = \frac{1}{2}m\omega^2(|x| - a)^2$$

as shown below:

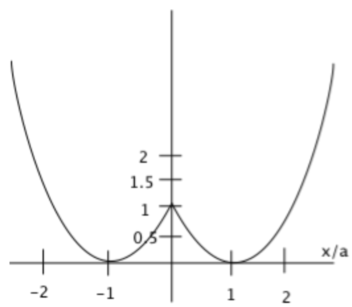

Figure 10.6: $n = 2$ Spectrum in Hydrogen

Argue that a good choice of trial wave functions are:

$$\psi_n^{\pm}(x) = u_n(x - a) \pm u_n(x + a)$$

where the $u_n(x)$ are the eigenfunctions for a harmonic potential centered at the origin.

(d) Using this show that the variational estimates of the energies are

$$E_n^{\pm} = \frac{A_n \pm B_n}{1 \pm C_n}$$

where

$$A_n = \int u_n(x - a)\hat{H}u_n(x - a)dx$$
$$B_n = \int u_n(x - a)\hat{H}u_n(x + a)dx$$
$$C_n = \int u_n(x + a)\hat{H}u_n(x - a)dx$$

(e) For a much larger than the ground state width, show that

$$\Delta E_0 = E_0^{(-)} - E_0^{(+)} \approx 2\hbar\omega\sqrt{\frac{2V_0}{\pi\hbar\omega}}e^{-2V_0/\hbar\omega}$$

where $V_0 = m\omega^2 a^2/2$. This is known as the ground *tunneling* splitting. Explain why?

(f) This approximation clearly breaks down as $a \to 0$. Think about the limits and sketch the energy spectrum as a function of a.

10.9.32 Variational Method 2

For a particle in a box that extends from $-a$ to $+a$, try the trial function (within the box)

$$\psi(x) = (x-a)(x+a)$$

and calculate E. There is no parameter to vary, but you still get an upper bound. Compare it to the true energy. Convince yourself that the singularities in ψ'' at $x = \pm a$ do not contribute to the energy.

10.9.33 Variational Method 3

For the attractive delta function potential

$$V(x) = -aV_0\delta(x)$$

use a Gaussian trial function. Calculate the upper bound on E_0 and compare it to the exact answer $-ma^2V_0^2/2h^2$.

10.9.34 Variational Method 4

For an oscillator choose

$$\psi(x) = \begin{cases} (x-a)^2(x+a)^2 & |x| \leq a \\ 0 & |x| > a \end{cases}$$

calculate $E(a)$, minimize it and compare to $\hbar\omega/2$.

10.9.35 Variation on a linear potential

Consider the energy levels of the potential $V(x) = g\,|x|$.

(a) By dimensional analysis, reason out the dependence of a general eigenvalue on the parameters $m = mass$, $\hbar$ and g.

(b) With the simple trial function

$$\psi(x) = c\theta(x+a)\theta(a-x)\left(1 - \frac{|x|}{a}\right)$$

compute (to the bitter end) a variational estimate of the ground state energy. Here both c and a are variational parameters.

(c) Why is the trial function $\psi(x) = c\theta(x+a)\theta(a-x)$ not a good one?

(d) Describe briefly (no equations) how you would go about finding a variational estimate of the energy of the first excited state.

10.9.36 Average Perturbation is Zero

Consider a Hamiltonian

$$H_0 = \frac{p^2}{2\mu} + V(r)$$

H_0 is perturbed by the spin-orbit interaction for a spin$= 1/2$ particle,

$$H' = \frac{A}{\hbar^2}\vec{S}\cdot\vec{L}$$

Show that the average perturbation of all states corresponding to a given term (which is characterized by a given L and S) is equal to zero.

10.9.37 3-dimensional oscillator and spin interaction

A spin$= 1/2$ particle of mass m moves in a spherical harmonic oscillator potential

$$U = \frac{1}{2}m\omega^2 r^2$$

and is subject to the interaction

$$V = \lambda\vec{\sigma}\cdot\vec{r}$$

Compute the shift of the ground state energy through second order.

10.9.38 Interacting with the Surface of Liquid Helium

An electron at a distance x from a liquid helium surface feels a potential

$$V(x) = \begin{cases} -K/x & x > 0 \\ \infty & x \le 0 \end{cases}$$

where K is a constant.

In Problem 8.7 we solved for the ground state energy and wave function of this system.

Assume that we now apply an electric field and compute the Stark effect shift in the ground state energy to first order in perturbation theory.

10.9.39 Positronium + Hyperfine Interaction

Positronium is a hydrogen atom but with a positron as the "nucleus" instead of a proton. In the nonrelativistic limit, the energy levels and wave functions are the same as for hydrogen, except for scaling due to the change in the reduced mass.

(a) From your knowledge of the hydrogen atom, write down the normalized wave function for the $1s$ ground state of positronium.

(b) Evaluate the root-mean-square radius for the $1s$ state in units of a_0. Is this an estimate of the physical diameter or radius of positronium?

(c) In the s states of positronium there is a contact *hyperfine* interaction

$$\hat{H}_{\text{int}} = -\frac{8\pi}{3}\vec{\mu}_e \cdot \vec{\mu}_p \delta(\vec{r})$$

where $\vec{\mu}_e$ and $\vec{\mu}_p$ are the electron and positron magnetic moments and

$$\vec{\mu} = \frac{ge}{2mc}\hat{\vec{S}}$$

Using first order perturbation theory compute the energy difference between the singlet and triplet ground states. Determine which lies lowest. Express the energy splitting in GHz. Get a number!

10.9.40 Two coupled spins

Two oppositely charged spin$-1/2$ particles (spins $\vec{s}_1 = \hbar\vec{\sigma}_1/2$ and $\vec{s}_2 = \hbar\vec{\sigma}_2/2$) are coupled in a system with a spin-spin interaction energy ΔE. The system is placed in a uniform magnetic field $\vec{B} = B\hat{z}$. The Hamiltonian for the spin interaction is

$$\hat{H} = \frac{\Delta E}{4}\vec{\sigma}_1 \cdot \vec{\sigma}_2 - (\vec{\mu}_1 + \vec{\mu}_2) \cdot \vec{B}$$

where $\vec{\mu}_j = g_j \mu_0 \vec{s}_j/\hbar$ is the magnetic moment of the j^{th} particle.

(a) If we define the 2-particle basis-states in terms of the 1-particle states by

$$|1\rangle = |+\rangle_1 |+\rangle_2 \quad , \quad |2\rangle = |+\rangle_1 |-\rangle_2 \quad , \quad |3\rangle = |-\rangle_1 |+\rangle_2 \quad , \quad |4\rangle = |-\rangle_1 |-\rangle_2$$

where

$$\sigma_{ix} |\pm\rangle_i = |\mp\rangle_i \quad , \quad \sigma_{ix} |\pm\rangle_i = \pm i |\mp\rangle_i \quad , \quad \sigma_{iz} |\pm\rangle_i = \pm |\pm\rangle_i$$

and

$$\sigma_{1x}\sigma_{2x} |1\rangle = \sigma_{1x}\sigma_{2x} |+\rangle_1 |+\rangle_2 = (\sigma_{1x} |+\rangle_1)(\sigma_{2x} |+\rangle_2) = |-\rangle_1 |-\rangle_2 = |4\rangle$$

then derive the results below.

The energy eigenvectors for the 4 states of the system, in terms of the eigenvectors of the $z-$component of the operators $\vec{\sigma}_{\mathrm{i}} = 2\vec{s}_i/\hbar$ are

$$|1'\rangle = |+\rangle_1 |+\rangle_2 = |1\rangle \quad , \quad |2'\rangle = d\,|-\rangle_1 |+\rangle_2 + c\,|+\rangle_1 |-\rangle_2 = d\,|3\rangle + c\,|2\rangle$$
$$|3'\rangle = c\,|-\rangle_1 |+\rangle_2 - dc\,|+\rangle_1 |-\rangle_2 = c\,|3\rangle - d\,|2\rangle \quad , \quad |4'\rangle = |-\rangle_1 |-\rangle_2 = |4\rangle$$

where

$$\vec{\sigma}_{\mathrm{zi}}\,|\pm\rangle_i = \pm\,|\pm\rangle_i$$

as stated above and

$$d = \frac{1}{\sqrt{2}}\left(1 - \frac{x}{\sqrt{1+x^2}}\right)^{1/2} \; , \; c = \frac{1}{\sqrt{2}}\left(1 + \frac{x}{\sqrt{1+x^2}}\right)^{1/2} \; , \; x = \frac{\mu_0 B(g_2 - g_1)}{\Delta E}$$

(b) Find the energy eigenvalues associated with the 4 states.

(c) Discuss the limiting cases

$$\frac{\mu_0 B}{\Delta E} \gg 1 \quad , \quad \frac{\mu_0 B}{\Delta E} \ll 1$$

Plot the energies as a function of the magnetic field.

10.9.41 Perturbed Linear Potential

A particle moving in one-dimension is bound by the potential

$$V(x) = \begin{cases} ax & x > 0 \\ \infty & x < 0 \end{cases}$$

where $a > 0$ is a constant. Estimate the ground state energy using first-order perturbation theory by the following method: Write $V = V_0 + V_1$ where $V_0(x) = bx^2$, $V_1(x) = ax - bx^2$ (for $x > 0$), where b is a constant and treat V_1 as a perturbation.

10.9.42 The ac-Stark Effect

Suppose an atom is perturbed by a monochromatic electric filed oscillating at frequency ω_L, $\vec{E}(t) = E_z \cos\omega_L t\hat{e}_z$ (such as from a linearly polarized laser), rather than the dc-field studied in the text. We know that such a field can be absorbed and cause transitions between the energy levels: we will systematically study this effect in Chapter 11. The laser will also cause a *shift* of energy levels of the unperturbed states, known alternatively as the *ac-Stark effect*, the *light shift*, and sometimes the *Lamp shift* (don't you love physics humor). In this problem, we will look at this phenomenon in the simplest case that the field is near to resonance between the ground state $|g\rangle$ and some excited state $|e\rangle$, $\omega_L \approx \omega_{eg} = (E_e - E_g)/\hbar$, so that we can ignore all other energy levels in the problem (the *two-level atom* approximation).

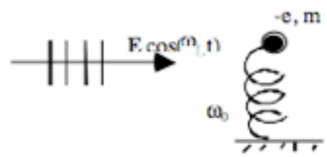

Figure 10.7: Lorentz Oscillator

(i) **The classical picture**. Consider first the *Lorentz oscillator* model of the atom - a charge on a spring - with natural resonance at ω_0. The Hamiltonian for the system is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 z^2 - \vec{d}\cdot\vec{E}(t)$$

where $d = -ez$ is the dipole.

(a) Ignoring damping of the oscillator, use Newton's Law to show that the induced dipole moment is

$$\vec{d}_{induced}(t) = \alpha\vec{E}(t) = \alpha E_z \cos\omega_L t$$

where

$$\alpha = \frac{e^2/m}{\omega_0^2 - \omega_L^2} \approx \frac{-e^2}{2m\omega_0\Delta}$$

is the polarizability with $\Delta = \omega_L - \omega_0$ the *detuning.*

(b) Use your solution to show that the total energy stored in the system is

$$H = -\frac{1}{2}d_{induced}(t)E(t) = -\frac{1}{2}\alpha E^2(t)$$

or the time average value of H is

$$bar H = -\frac{1}{4}\alpha E_z^2$$

Note the factor of 1/2 arises because energy is required to *create* the dipole.

(ii) **The quantum picture**. We consider the two-level atom described above. The Hamiltonian for this system can be written in a time independent form (equivalent to the time-averaging done in the classical case).

$$\hat{H} = \hat{H}_{atom} + \hat{H}_{int}$$

where $\hat{H}_{atom} = -\hbar\Delta\left|e\right\rangle\left\langle e\right|$ is the *unperturbed* atomic Hamiltonian and $\hat{H}_{int} = -\frac{\hbar\Omega}{2}\left(\left|e\right\rangle\left\langle g\right| + \left|g\right\rangle\left\langle e\right|\right)$ is the dipole-interaction with $\hbar\Omega = \left\langle e\right|\vec{d}\left|g\right\rangle\cdot\vec{E}$.

(a) Find the *exact* energy eigenvalues and eigenvectors for this simple two dimensional Hilbert space and plot the levels as a function of Δ. These are known as the atomic *dressed states.*

(b) Expand your solution in (a) to lowest nonvanishing order in Ω to find the perturbation to the energy levels. Under what conditions is this expansion valid?

(c) Confirm your answer to (b) using perturbation theory. Find also the mean induced dipole moment (to lowest order in perturbation theory), and from this show that the atomic polarizability, defined by $\langle \vec{d} \rangle = \alpha \vec{E}$ is given by

$$\alpha = -\frac{|\langle e|\,\vec{d}\,|g\rangle|^2}{\hbar\Delta}$$

so that the second order perturbation to the ground state is $E_g^{(2)} = -\alpha E_z^2$ as in part (b).

(d) Show that the ratio of the polarizability calculated classically in (b) and the quantum expression in (c) has the form

$$f = \frac{\alpha_{quantum}}{\alpha_{classical}} = \frac{|\langle e|\,z\,|g\rangle|^2}{(\Delta z^2)_{SHO}}$$

where $\left(\Delta z^2\right)_{SHO}$ is the SHO zero point variance. This is also known as the oscillator strength.

We see that in lowest order perturbation theory an atomic resonance looks just like a harmonic oscillator with a correction factor given by the oscillator strength and off-resonance harmonic perturbations cause energy level shifts as well as absorption and emission(Chapter 11).

10.9.43 Light-shift for multilevel atoms

We found the ac-Stark (light shift) for the case of a two-level atom driven by a monchromatic field. In this problem we want to look at this phenomenon in a more general context, including arbitrary polarization of the electric field and atoms with multiple sublevels.

Consider then a general monochromatic electric field $\vec{E}(\vec{x},t) = \Re(\vec{E}(\vec{x})e^{-i\omega_L t})$, driving an atom near resonance on the transition $|g; J_g\rangle \to |e; J_e\rangle$, where the ground and excited manifolds are each described by some total angular momentum J with degeneracy $2J+1$. The generalization of the ac-Stark shift is now the light-shift operator acting on the $2J_g+1$ dimensional ground manifold:

$$\hat{V}_{LS}(\vec{x}) = -\frac{1}{4}\vec{E}^*(\vec{x}) \cdot \hat{\overset{\leftrightarrow}{\alpha}} \cdot \vec{E}(\vec{x})$$

Here,

$$\hat{\overleftrightarrow{\alpha}} = -\frac{\hat{\vec{d}}_{ge}\hat{\vec{d}}_{eg}}{\hbar\Delta}$$

is the atomic polarizability tensor operator, where $\hat{\vec{d}}_{eg} = \hat{P}_e\hat{\vec{d}}\hat{P}_g$ is the dipole operator, projected between the ground and excited manifolds; the projector onto the excited manifold is

$$\hat{P}_e = \sum_{M_e=-J_e}^{J_e} |e; J_e, M_e\rangle \langle e; J_e, M_e|$$

and similarly for the ground manifold.

(a) By expanding the dipole operator in the spherical basis$(\pm, 0)$, show that the polarizability operator can be written

$$\hat{\overleftrightarrow{\alpha}} = \tilde{\alpha}\left(\begin{array}{l} \sum_{q,M_g} \left|C_{M_g}^{M_g+q}\right|^2 \vec{e}_q\, |g, J_g, M_g\rangle \langle g, J_g, M_g|\, \vec{e}_q^{\;*} \\ \quad + \sum_{q\neq q', M_g} C_{M_g+q-q'}^{M_g+q}\, C_{M_g}^{M_g+q}\, \vec{e}_{q'}\, |g, J_g, M_g+q-q'\rangle \langle g, J_g, M_g|\, \vec{e}_q^{\;*} \end{array}\right)$$

where

$$\tilde{\alpha} = -\frac{|\langle e; J_e \,\|d\|\, g; J_g\rangle|^2}{\hbar\Delta}$$

and

$$C_{M_g}^{M_e} = \langle J_e M_e \,|\, 1q J_g M_g\rangle$$

Explain physically, using dipole selection rules, the meaning of the expression for $\hat{\overleftrightarrow{\alpha}}$.

(b) Consider a polarized plane wave, with complex amplitude of the form $\vec{E}(\vec{x}) = E_1\vec{\varepsilon}_L e^{i\vec{k}\cdot\vec{x}}$ where E_1 is the amplitude and $\vec{\varepsilon}_L$ the polarization (possibly complex). For an atom driven on the transition $|g; J_g = 1\rangle \to |e; J_e = 2\rangle$ and the cases (i) linear polarization along z, (ii) positive helicity polarization, (iii) linear polarization along x, find the eigenvalues and eigenvectors of the light-shift operator. Express the eigenvalues in units of

$$V_1 = -\frac{1}{4}\tilde{\alpha}|E_1|^2.$$

Please comment on what you find for cases (i) and (iii). Repeat for $|g; J_g = 1/2\rangle \to |e; J_e = 3/2\rangle$ and comment.

(c) A deeper insight into the light-shift potential can be seen by expressing the polarizability operator in terms of irreducible tensors. Verify that the total light shift is the sum of scalar, cvector, and rank-2 irreducible tensor interactions,

$$\hat{V}_{LS} = -\frac{1}{4}\left(|\vec{E}(\vec{x})|^2\alpha^{\hat{(0)}} + (\vec{E}^*(\vec{x}) \times \vec{E}(\vec{x}) \cdot \alpha^{\hat{(1)}} + \vec{E}^*(\vec{x}) \cdot \alpha^{\hat{(2)}} \cdot \vec{E}(\vec{x})\right)$$

where

$$\alpha^{\hat{(0)}} = \frac{\hat{\vec{d}}_{ge} \cdot \hat{\vec{d}}_{eg}}{-3\hbar\Delta} \quad , \quad \alpha^{\hat{(1)}} = \frac{\hat{\vec{d}}_{ge} \times \hat{\vec{d}}_{eg}}{-2\hbar\Delta}$$

and

$$\alpha^{\hat{(2)}}{}_{ij} = \frac{1}{-\hbar\Delta}\left(\frac{\hat{\vec{d}}^{i}_{ge}\hat{\vec{d}}^{j}_{ge} + \hat{\vec{d}}^{j}_{ge}\hat{\vec{d}}^{i}_{ge}}{2} - \alpha^{\hat{(0)}}\delta_{ij}\right)$$

(d) For the particular case of $|g; J_g = 1/2\rangle \to |e; J_e = 3/2\rangle$, show that the rank-2 tensor part vanishes. Show that the light-shift operator can be written in a basis independent form of a scalar interaction (independent of sublevel), plus an effective Zeeman interaction for a fictitious B-field interacting with the spin$-1/2$ ground state,

$$\hat{V}_{LS} = V_0(\vec{x})\hat{I} + \vec{B}_{fict}(\vec{x}) \cdot \hat{\vec{\sigma}}$$

where

$$V_0(\vec{x}) = \frac{2}{3}U_1|\vec{\varepsilon}_L(\vec{x})|^2 \to \text{ proportional to field intensity}$$

and

$$\vec{B}_{fict}(\vec{x}) = \frac{1}{3}U_1\left(\frac{\vec{\varepsilon}_L{}^*(\vec{x}) \times \vec{\varepsilon}_L(\vec{x})}{i}\right) \to \text{ proportional to field ellipticity}$$

and we have written $\vec{E}(\vec{x}) = E_1\vec{\varepsilon}_L(\vec{x})$. Use this form to explain your results from part (b) on the transition $|g; J_g = 1/2\rangle \to |e; J_e = 3/2\rangle$.

10.9.44 A Variational Calculation

Consider the one-dimensional box potential given by

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

Use the variational principle with the trial function

$$\psi(x) = |a|^\lambda - |x|^\lambda$$

where λ is a variational parameter. to estimate the ground state energy. Compare the result with the exact answer.

10.9.45 Hyperfine Interaction Redux

An important effect in the study of atomic spectra is the so-called *hyperfine interaction* – the magnetic coupling between the electron spin and the nuclear spin. Consider Hydrogen. The hyperfine interaction Hamiltonian has the form

$$\hat{H}_{HF} = g_s g_i \mu_B \mu_N \frac{1}{r^3}\hat{s} \cdot \hat{i}$$

where $\hat{s}$ is the electron's spin$-1/2$ angular momentum and $\hat{i}$ is the proton's spin$-1/2$ angular momentum and the appropriate g-factors and magnetons are given.

(a) In the absence of the hyperfine interaction, but including the electron and proton spin in the description, what is the degeneracy of the ground state? Write all the quantum numbers associated with the degenerate sublevels.

(b) Now include the hyperfine interaction. Let $\hat{f} = \hat{i} + \hat{s}$ be the total spin angular momentum. Show that the ground state manifold is described with the good quantum numbers $|n = 1, \ell = 0, s = 1/2, i = 1/2, f, m_f\rangle$. What are the possible values of f and m_f?

(c) The perturbed $1s$ ground state now has hyperfine splitting. The energy level diagram is sketched below.

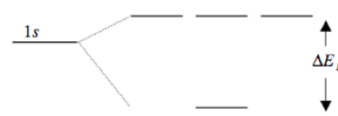

Figure 10.8: Hyperfine Splitting

Label all the quantum numbers for the four sublevels shown in the figure.

(d) Show that the energy level splitting is

$$\Delta E_{HF} = g_s g_i \mu_B \mu_N \langle \frac{1}{r^3} \rangle_{1s}$$

Show numerically that this splitting gives rise to the famous 21 cm radio frequency radiation used in astrophysical observations.

10.9.46 Find a Variational Trial Function

We would like to find the ground-state wave function of a particle in the potential $V = 50(e^{-x} - 1)^2$ with $m = 1$ and $\hbar = 1$. In this case, the true ground state energy is known to be $E_0 = 39/8 = 4.875$. Plot the form of the potential. Note that the potential is more or less quadratic at the minimum, yet it is skewed. Find a variational wave function that comes within 5% of the true energy. OPTIONAL: How might you find the exact analytical solution?

10.9.47 Hydrogen Corrections on 2s and 2p Levels

Work out the first-order shifts in energies of $2s$ and $2p$ states of the hydrogen atom due to relativistic corrections, the spin-orbit interaction and the so-called

Darwin term,

$$-\frac{p^4}{8m_e^3c^2} + g\frac{1}{4m_e^2c^2}\frac{1}{r}\frac{dV_c}{dr}(\vec{L}\cdot\vec{S}) + \frac{\hbar^2}{8m_e^2c^2}\nabla^2 V_c \ , \ \ V_c = -\frac{Ze^2}{r}$$

where you should be able to show that $\nabla^2 V_c = 4\pi\delta(\vec{r})$. At the end of the calculation, take $g = 2$ and evaluate the energy shifts numerically.

10.9.48 Hyperfine Interaction Again

Show that the interaction between two magnetic moments is given by the Hamiltonian

$$H = -\frac{2}{3}\mu_0(\vec{\mu}_1\cdot\vec{\mu}_2)\delta(\vec{x}-\vec{y}) - \frac{\mu_0}{4\pi}\frac{1}{r^3}\left(3\frac{r_i r_j}{r^2} - \delta_{ij}\right)\mu_1^i\mu_2^j$$

where $r_i = x_i - y_i$. (NOTE: Einstein summation convention used above). Use first-order perturbation to calculate the splitting between $F = 0, 1$ levels of the hydrogen atoms and the corresponding wavelength of the photon emission. How does the splitting compare to the temperature of the cosmic microwave background?

10.9.49 A Perturbation Example

Suppose we have two spin$-1/2$ degrees of freedom, A and B. Let the initial Hamiltonian for this joint system be given by

$$H_0 = -\gamma B_z\left(S_z^A \otimes I^B + I^A \otimes S_z^B\right)$$

where I^A and I^B are identity operators, S_z^A is the observable for the $z-$component of the spin for the system A, and S_z^B is the observable for the $z-$component of the spin for the system B. Here the notation is meant to emphasize that both spins experience the same magnetic field $\vec{B} = B_z\hat{z}$ and have the same gyromagnetic ratio γ.

(a) Determine the energy eigenvalues and eigenstates for H_0

(b) Suppose we now add a perturbation term $H_{total} = H_0 + W$, where

$$W = \lambda\vec{S}^A\cdot\vec{S}^B = \lambda\left(S_x^A\otimes S_x^B + S_y^A\otimes S_y^B + S_z^A\otimes S_z^B\right)$$

Compute the first-order corrections to the energy eigenvalues.

10.9.50 More Perturbation Practice

Consider two spi$-1/2$ degrees of freedom, whose joint pure states can be represented by state vectors in the tensor-product Hilbert space $mathcalH_{AB} = mathcalH_A \otimes mathcalH_B$, where $mathcalH_A$ and $mathcalH_B$ are each two-dimensional. Suppose that the initial Hamiltonian for the spins is

$$H_0 = \left(-\gamma_A B_z S_z^A\right)\otimes I^B + I^A \otimes\left(-\gamma_B B_z S_z^B\right)$$

(a) Compute the eigenstates and eigenenergies of H_0, assuming $\gamma_A \neq \gamma_B$ and that the gyromagnetic ratios are non-zero. If it is obvious to you what the eigenstates are, you can just guess them and compute the eigenenergies.

(b) Compute the first-order corrections to the eigenstates under the perturbation

$$W = \alpha S_x^A \otimes S_x^B$$

where α is a small parameter with appropriate units.

Chapter 11

Time-Dependent Perturbation Theory

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

$$V(x, y, z) = k\left(x^2 + y^2 + z^2\right) \tag{11.-1}$$

(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

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

11.5.10 Time Evolution Operator

A one-dimensional anharmonic oscillator is given by the Hamiltonian

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

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, or solve the problem exactly.

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

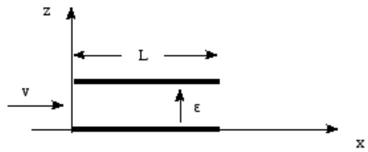

Figure 11.1: Hydrogen beam between parallel plates

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.
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:

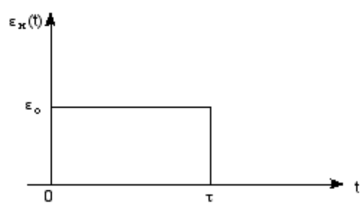

Figure 11.2: Electric Field

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!)

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

At $t = -\infty$, the oscillator is known to be in the ground state. Using time-dependent 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 $\tau >> 1/\omega$, 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

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

(a) What is the new ground state energy?

(b) Assuming that the field is switched on in a time much faster than $1/\omega$, 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

$$\hat{V}_1 = \frac{1}{2}k\,|-\rangle\langle-| \otimes |\vec{r}|^2$$

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

$$\hat{W} = \hbar\Omega \left(|-\rangle \langle+| + |+\rangle \langle-| \otimes |\vec{r}|^2 \right) \otimes \hat{I}^{CM}$$

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

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

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

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

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

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 Schrodinger equation with this Hamiltonian and find the corresponding eigenvalue. Assume here that $\alpha = m\omega/\hbar$, $\omega = sqrtk/m$ 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 $\hat{a}^+$ 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

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

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

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

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 Schrodinger equation and the sudden approximation to compute the subsequent evolution of $|\Psi(t)\rangle$ and determine the function

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

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

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

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

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

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:

$$\begin{aligned}
|E_0\rangle &= |g\rangle \otimes |0\rangle \\
|E_{1+}\rangle &= \frac{1}{\sqrt{2}}\left(|g\rangle \otimes |1\rangle + |e\rangle \otimes |0\rangle\right) \\
|E_{1-}\rangle &= \frac{1}{\sqrt{2}}\left(|g\rangle \otimes |1\rangle - |e\rangle \otimes |0\rangle\right) \\
|E_{2+}\rangle &= \frac{1}{\sqrt{2}}\left(|g\rangle \otimes |2\rangle + |e\rangle \otimes |1\rangle\right) \\
|E_{2-}\rangle &= \frac{1}{\sqrt{2}}\left(|g\rangle \otimes |2\rangle - |e\rangle \otimes |1\rangle\right)
\end{aligned}$$

The 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

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

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

12.9 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 anti-symmetric. 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

$$V_a(r) = \begin{cases} 0 & \text{for } r < a \\ V_0 & \text{for } r > a \end{cases} \quad , \quad V_b(r) = \begin{cases} 0 & \text{for } r < b \\ V_0 & \text{for } r > b \end{cases}$$

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

$$\langle 1/r \rangle_{n\ell m} = \frac{me^2}{n^2\hbar^2} = \frac{1}{n^2 a_0}$$

We note (for later use) that

$$E(\lambda) = E^{(0)} + E^{(1)} + ... = E(\lambda = 0) + \lambda \left(\frac{dE}{d\lambda} \right)_{\lambda=0} + ...$$

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), $\left\langle \vec{p}^2/2\mu \right\rangle_{n\ell m}$ 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 $\left\langle \lambda/r^2 \right\rangle_{n\ell m}$. 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

$$E(\ell') = -\frac{mZ^2e^4}{2\hbar^2(k+\ell'+1)^2} = E(\lambda) = E^{(0)} + E^{(1)} + ...$$

Then show that

$$\begin{aligned} \left\langle \lambda/r^2 \right\rangle_{n\ell m} &= E^{(1)} \lambda \left(\frac{dE}{d\lambda} \right)_{\lambda=0} = \lambda \left(\frac{dE}{d\ell'} \right)_{\ell'=\ell} \left(\frac{d\ell'}{d\lambda} \right)_{\ell'=\ell} \\ &= \frac{\lambda}{n^3 a_0^2 (\ell + 1/2)} \end{aligned}$$

or

$$\left\langle 1/r^2 \right\rangle_{n\ell m} = \frac{1}{n^3 a_0^2 (\ell + 1/2)}$$

(d) Finally consider $\left\langle \lambda/r^3 \right\rangle_{n\ell m}$. 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

$$-\frac{\hbar^2}{2m} \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right)$$

as

$$\frac{p_r^2}{2m}$$

Now show that

$$\langle [H, p_r] \rangle = 0$$

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

$$\left\langle 1/r^3 \right\rangle_{n\ell m} = \frac{Z^3}{n^3 a_0^3 \ell(\ell+1)(\ell+1/2)}$$

12.9.5 Hund's rule

Explain on the basis of Hunds rules why the ground state of carbon is $^3P_0$ and that of oxygen is $^3P_2$.

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

$$g_p = 2 \times (2.792847337 \pm 0.000000029)$$

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 $|1/2, 1/2\rangle$ 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 uud 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

$$\hat{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m_1\omega^2 x_1^2 + \frac{1}{2}m_2\omega^2 x_2^2 + \frac{1}{2}K\left(x_1 - x_2\right)^2$$

(a) Find the exact solutions.

(b) Sketch the spectrum in weak coupling limit $K << \mu\omega^2$ where $\mu =$ reduced mass.

12.9.10 LS versus JJ coupling

Consider a multielectron atom whose electron configuration is

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p 4d$$

(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 J lies 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 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.

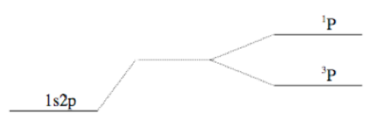

Figure 12.1: Fermi-Pauli Splittings

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.

(b) Without the spin-orbit interaction, good quantum numbers for the angular momentum degrees of freedom are $|LM_L SM_S\rangle$. What are the good quantum numbers with spin-orbit present?

(c) The energy level diagram including spin-orbit corrections is sketched below.

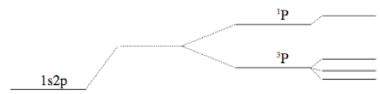

Figure 12.2: Including Spin-Orbit

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

13.3 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):

$$\left[-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{2mC}{\hbar^2 r^4} \right] R_{\ell=0}^{inside}(r) = 0$$

By making the transformations

$$R(r) = \frac{1}{\sqrt{r}}\varphi(r) \quad , \quad r = \frac{i}{\hbar}\frac{\sqrt{2mC}}{x}$$

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 o fmatching 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_0a^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

$$V(r) = \begin{cases} 0 & r > r_0 \\ \infty & r < r_0 \end{cases} \tag{13.-7}$$

where $kr_0 \ll 1$. Write the radial Schrodinger 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:

$$\hat{H} = \begin{pmatrix} E_0 & A \\ A & E_0 \end{pmatrix}$$

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 $|I\rangle$, that is, $|\psi(0)\rangle = |I\rangle$. 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?

(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
?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.

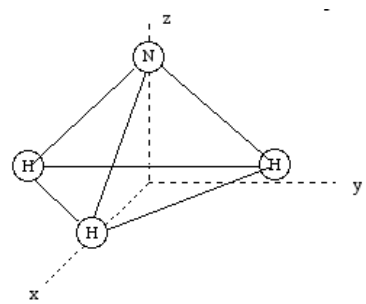

Figure 13.1: Ammonia Molecule

(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

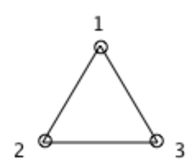

Figure 13.2: A Molecule

The eigenstates of the molecule can be written as linear combinations of the atomic states $|\alpha_i\rangle$, $i = 1, 2, 3$, such that

$$\langle\alpha_i|\hat{H}|\alpha_j\rangle = \begin{cases} \varepsilon & \text{if } i = j \\ -\beta & \text{if } i \neq j \end{cases} \tag{13.-11}$$

where $\hat{H}$ is the Hamiltonian and ε, $\beta > 0$. Now define an operator $\hat{R}$ such that

$$\hat{R}|\alpha_1\rangle = |\alpha_2\rangle \quad , \quad \hat{R}|\alpha_2\rangle = |\alpha_3\rangle \quad , \quad \hat{R}|\alpha_3\rangle = |\alpha_1\rangle$$

(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

$$V(\vec{r}) = \begin{cases} V_1 & 0 < |\vec{r}| < R_1 \\ V_2 & R_1 < |\vec{r}| < R_2 \end{cases} \tag{13.-12}$$

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 $V_1 = V_2 \to V_0$.

(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., $qR_2 \to 0$, $qR_2 \sim 1$, $qR_2 \gg 1$). 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

$$\langle r^2 \rangle = \frac{12}{b^2}$$

(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

$$V(x) = \begin{cases} V_0 & |x| < a/2 \\ 0 & |x| > a/2 \end{cases} \tag{13.-15}$$

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

$$V(x) = \begin{cases} 0 & r > b \\ \infty & r \leq b \end{cases} \tag{13.-15}$$

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

$$V(x) = \begin{cases} 0 & r > b \\ = V_0 & r \leq b \end{cases} \tag{13.-15}$$

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

$$V(r) = -Ze^2\int\frac{\rho_T(\overleftarrow{r}')d^3\vec{r}'}{|\vec{r}-\vec{r}'|}$$

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.

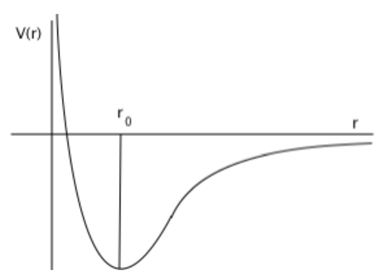

Figure 13.3: Lennard-Jones Potential

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

$$\begin{aligned} E_n^{(2)} &= \frac{\xi^2\hbar^2}{m^3\omega^4}\left[\frac{(n-2)(n-1)(n)}{3} + \frac{(n+3)(n+2)(n+1)}{-3} + \frac{9n^3}{1} + \frac{9(n+1)^3}{-1}\right] \\ &= -\frac{\xi^2\hbar^2}{m^3\omega^4}\left[\frac{15}{4}(n+1/2)^2 + \frac{7}{16}\right] \end{aligned}$$

(f) Consider carbon C-C bonds take Lennard-Jones parameters $C_6 = 15.2\ eV\ \text{Å}^6$ and $C_{12} = 2.4 \times 10^4\ eV\ \text{Å}^{12}$. Plot the potential and the energy levels from the ground to second excited state including the anharmonic shifts.

13.3.22 Covalent Bonds - Diatomic Hydrogen

Consider the simplest neutral molecule, diatomic hydrogen H_2, consisting of two electrons and two protons.

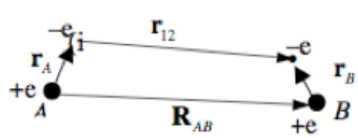

Figure 13.4: Diatomic Molecule

(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 inter-nuclear 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 15

States and Measurement

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).

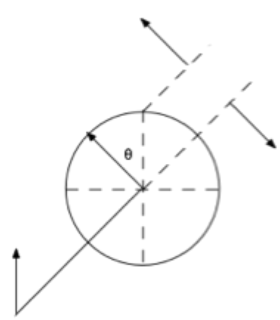

Figure 15.1: Tilted Stern-Gerlach Setup

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.

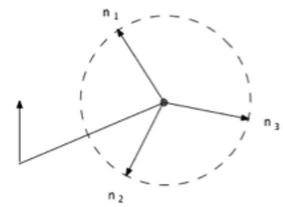

Figure 15.2: Variable Orientation Stern-Gerlach Setup

More specifically, assume that it can have the three different directions

$$\hat{n}_1 = \hat{n} = \cos\theta\hat{z} - \sin\theta\hat{x}$$
$$\hat{n}_2 = \cos\left(\theta + \tfrac{2}{3}\pi\right)\hat{z} - \sin\left(\theta + \tfrac{2}{3}\pi\right)\hat{x}$$
$$\hat{n}_3 = \cos\left(\theta + \tfrac{4}{3}\pi\right)\hat{z} - \sin\left(\theta + \tfrac{4}{3}\pi\right)\hat{x}$$

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 $|0.0\rangle$. 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.

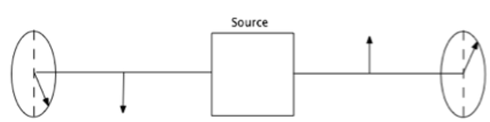

Figure 15.3: EPR Stern-Gerlach Setup

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

$$|1,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{(1)}|\downarrow\rangle_{(2)} - |\downarrow\rangle_{(1)}|\uparrow\rangle_{(2)}\right) \tag{15.-4}$$

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

$$|\psi\rangle\,|0\rangle = \frac{1}{2}\left(|0\rangle\,|\psi\rangle + |1\rangle\,|\psi'\rangle + |2\rangle\,|\psi''\rangle + |3\rangle\,|\psi'''\rangle\right)$$

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:

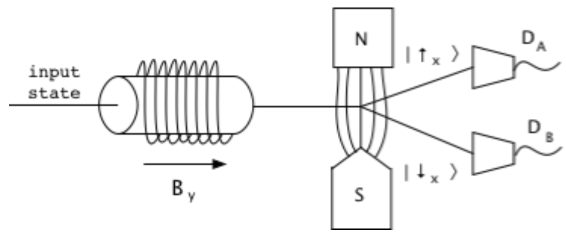

Figure 15.4: EPR Stern-Gerlach Setup

?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,

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle + |\downarrow_z\rangle\right)$$

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

$$\hat{\rho} = \frac{1}{2}\left(|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\downarrow_z|\right)$$

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

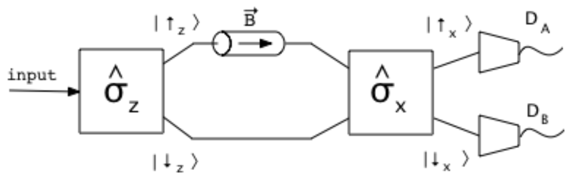

Figure 15.5: Spin-Interferometer Setup

path, 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:

$$(i)\ \ |\uparrow_z\rangle \quad , \quad (ii)\ |\downarrow_z\rangle \quad , \quad (iii)\ \ |\uparrow_x\rangle \quad , \quad (iv)\ \ |\downarrow_x\rangle$$

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

$$P_{D_A} = Tr\left[\left|\uparrow_x\right\rangle\left\langle\uparrow_x\right|\hat{\rho}\right] = \sum_i p_i \left|\left\langle\uparrow_x \mid \psi_i\right\rangle\right|^2$$

where $\left|\left\langle\uparrow_x \mid \psi_i\right\rangle\right|^2$ = 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:

$(i)\ \ \hat{\rho} = \frac{1}{2}\left|\uparrow_z\right\rangle\left\langle\uparrow_z\right| + \frac{1}{2}\left|\downarrow_z\right\rangle\left\langle\downarrow_z\right| \quad , \quad (ii)\ \ \hat{\rho} = \frac{1}{2}\left|\uparrow_x\right\rangle\left\langle\uparrow_x\right| + \frac{1}{2}\left|\downarrow_x\right\rangle\left\langle\downarrow_x\right| \quad ,$

$(iii)\ \ \hat{\rho} = \frac{1}{3}\left|\uparrow_z\right\rangle\left\langle\uparrow_z\right| + \frac{2}{3}\left|\downarrow_z\right\rangle\left\langle\downarrow_z\right|$

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:

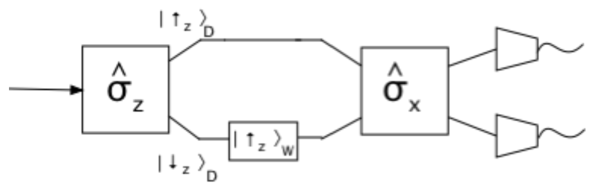

Figure 15.6: Spin-Interferometer Setup

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 $|{\uparrow_z}\rangle_W \to |{\downarrow_z}\rangle_W$, 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

$$|{\uparrow_z}\rangle_D |{\uparrow_z}\rangle_W \to |{\uparrow_z}\rangle_D |{\uparrow_z}\rangle_W \qquad |{\downarrow_z}\rangle_D |{\uparrow_z}\rangle_W \to |{\uparrow_z}\rangle_D |{\downarrow_z}\rangle_W$$

(a) The electron D is initially prepared in the state $|{\uparrow_x}\rangle_D = \left(|{\uparrow_z}\rangle_D + |{\downarrow_z}\rangle_D\right)/\sqrt{2}$. 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,

$$\hat{\rho}_D = \frac{1}{2}|{\uparrow_z}\rangle_D\, {}_D\langle{\uparrow_z}| + \frac{1}{2}|{\downarrow_z}\rangle_D\, {}_D\langle{\downarrow_z}|$$

This can be done by calculating

$$\text{Prob}(m_D) = \sum_{m_W} |\langle m_D, m_W \mid \Psi_{DW}\rangle|^2$$

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

$$\begin{aligned}\hat{\rho}_D = &\frac{1}{2}\,|\uparrow_z\rangle_D\,{}_D\langle\uparrow_z| + \frac{1}{2}\,|\downarrow_z\rangle_D\,{}_D\langle\downarrow_z| \\ &+ \cos(\theta/2)\,|\uparrow_z\rangle_D\,{}_D\langle\downarrow_z| + \sin(\theta/2)\,|\downarrow_z\rangle_D\,{}_D\langle\uparrow_z|\end{aligned}$$

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

$$\rho = \frac{1}{2}\left(|LL\rangle\langle LL| + |RR\rangle\langle RR|\right)$$

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 light-year 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

$$\rho = \frac{1}{2}\left(|LL\rangle + |RR\rangle\right)\left(\langle LL| + \langle RR|\right)$$

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 $\{|\nu\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,, \left|\nu^{\perp}\right\rangle\}$, 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 $\left|\nu^{\perp}\right\rangle$ 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

$$Pr[qubit\,was\ |0\rangle]Pr[|\nu\rangle\ |qubit\,was\ |0\rangle]+Pr[qubit\,was\ |\psi\rangle]Pr[\left|\nu^{\perp}\right\rangle |qubit\,was\ |\psi\rangle]$$

where, e.g.

$$Pr[|\nu\rangle\ |qubit\,was\ |0\rangle] = |\,\langle \nu\mid 0\rangle\,|^2$$

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

16.10 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).

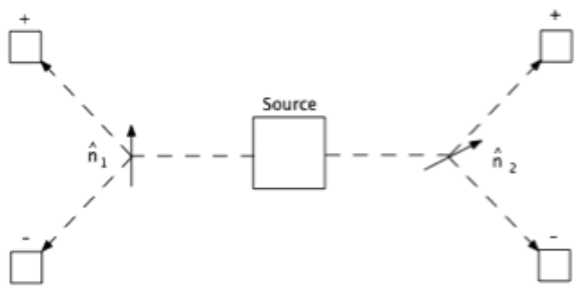

Figure 16.1: EPR Stern-Gerlach Setup

(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 it is meaningful value to the spin of a particle 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*

$$\left| \left\langle \sigma^{(12)}(\varphi) \right\rangle - \left\langle \sigma^{(12)}(\varphi') \right\rangle \right| \leq 1 + \left| \left\langle \sigma^{(12)}(\varphi - \varphi') \right\rangle \right|$$

(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) $\rho(\lambda) \geq 0$

(b) $\int d\lambda \rho(\lambda) = 1$

(c) $-1 \leq C(\hat{a},\lambda) \leq 1$, $-1 \leq C(\hat{b},\lambda) \leq 1$

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 $C(\hat{a},\hat{b}) = 2\left(\hat{a}\cdot\hat{b}\right)^2 - 1$

(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

17.7 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

$$A_1(\vec{r}) = -\frac{B}{2} x_2 \quad , \quad A_2(\vec{r}) = \frac{B}{2} x_1$$

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

Consdider 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
$$\langle q = 0, t_f \,|\, q = 0, t_i \rangle$$
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

18.7 Problems

18.7.1 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.

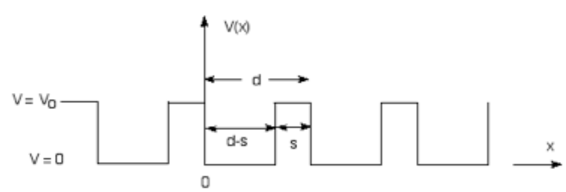

Figure 18.1: Piecewise Constant Potential - 1 Atom per Primitive Cell

(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.

(b) For $s = d/3$, what are the magnitudes of the lowest six band gaps in the weak binding limit?

18.7.2 Piecewise Constant Potential Energy Two Atoms per Primitive Cell

Consider a one-dimensional crystal with two atoms per primitive unit cell as shown below.

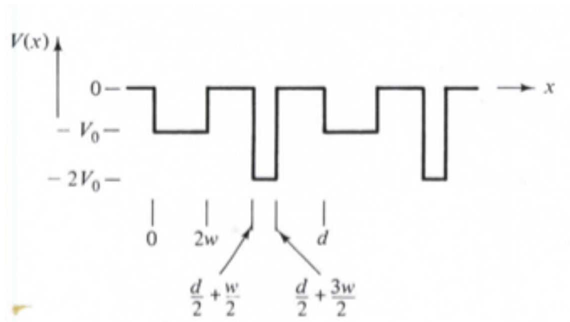

Figure 18.2: Piecewise Constant Potential - 2 Atoms per Primitive Cell

(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 anything 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.

18.7.3 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.

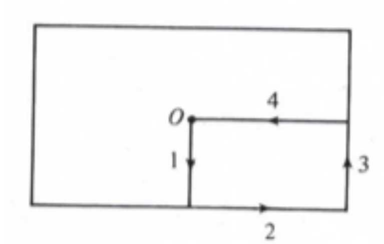

Figure 18.3: Paths in the First Brillouin Zone

(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.

18.7.4 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 $\vec{k}$ space (starting at $\vec{k} = 0$) along the path in the first Brillouin zone shown in the figure below. Do this for the six lowest bands in both the free-electron and weak-binding approximations (assuming (incorrectly) that all degeneracies are absent in the latter case).

(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 $\eta = 1$ *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

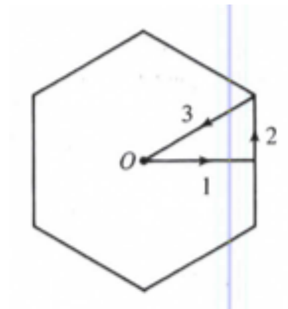

Figure 18.4: Paths in the First Brillouin Zone

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?

18.7.5 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.

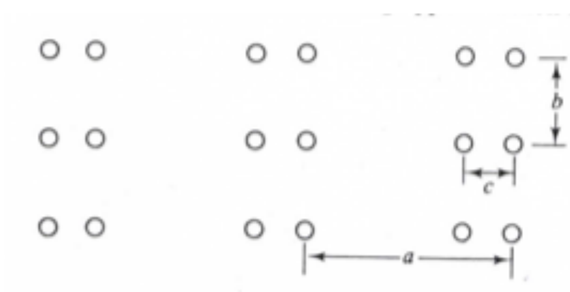

Figure 18.5: 2-Dimensional Crystal - Rectangular Bravais Lattice with 2 Atoms per Primitive Unit Cell

(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.

18.7.6 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).

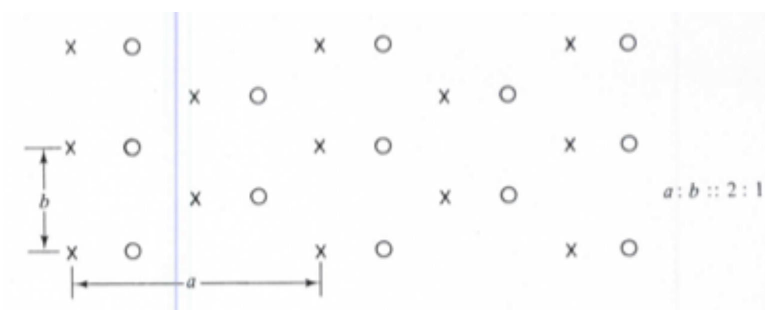

Figure 18.6: 2-Dimensional Crystal - Centered Rectangular Bravais Lattice with 2 Atoms per Primitive Unit Cell

Chapter 19

Second Quantization

19.9 Problems

19.9.1 Bogoliubov Transformations

Consider a Hamiltonian for Bosonic operators $\hat{b}_k^+, \hat{b}_k$ of the form

$$\hat{H} = E(k)\hat{b}_k^+\hat{b}_k + A(k)\left[\hat{b}_k^+\hat{b}_{-k}^+ + \hat{b}_k\hat{b}_{-k}\right]$$

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

$$\hat{H} = \sum_k \varepsilon(k)\hat{a}_k^+\hat{a}_k + \frac{1}{2V}\sum_q V_q \sum_{p,k} \hat{a}_{p+q}^+\hat{a}_{k-q}^+\hat{a}_k\hat{a}_p$$

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:

$$\hat{b}_k^+ e^{i\theta} = \hat{c}_k \cosh\phi_k + \hat{c}_{-k}^+ \sinh\phi_k$$

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

$$\hat{c}_k = \tilde{b}_k \cosh\phi_k - \tilde{b}_{-k}^+ \sinh\phi_k$$

where $\tilde{b}_k = \hat{b}_k e^{-i\theta}$. Use

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + ...$$

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 $\hat{K}$ in the Bogoliubov approximation is $|GS\rangle = U(\phi)\left|\tilde{0}\right\rangle$ where $\left|\tilde{0}\right\rangle$ is the vacuum of the operators $\tilde{b}_k : \tilde{b}_k\left|\tilde{0}\right\rangle = 0$ for all k. Argue that $|GS\rangle$ is a linear superposition of states with a pair of momenta $\vec{k}, -\vec{k}$ 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 $\hat{H}$:

$$\hat{H} = \int d^3x\, \hat{\psi}^+(\vec{x}) \left(-\frac{\hbar^2\nabla^2}{2m} + U(\vec{x})\right) \hat{\psi}(\vec{x}) + \frac{1}{2}\int\int d^3x\, d^3y\, \hat{\psi}^+(\vec{x})\hat{\psi}^+(\vec{y})V(\vec{x}-\vec{y})\hat{\psi}(\vec{y})\hat{\psi}(\vec{x})$$

(a) 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 $\hat{\psi}(\vec{x}) \to \psi(\vec{x}) + \hat{\eta}(\vec{x})$ where $\psi(\vec{x})$ is the solution to the Gross-Pitaevskii equation and write $\hat{K}$ up to quadratic order in $\hat{\eta}(\vec{x}), \hat{\eta}^+(\vec{x})$. Show that terms linear in $\hat{\eta}(\vec{x}), \hat{\eta}^+(\vec{x})$ are cancelled by $\psi(\vec{x})$ being a solution to the Gross-Pitaevskii equation.

(c) Introduce the Bogoliubov transformation:

$$\hat{\phi}(\vec{x}) = u(\vec{x})\hat{\eta}(\vec{x}) + v(\vec{x})\hat{\eta}^+(\vec{x}) \;\;,\;\; \hat{\phi}^+(\vec{x}) = u^*(\vec{x})\hat{\eta}^+(\vec{x}) + v^*(\vec{x})\hat{\eta}(\vec{x})$$

Show that $\left[\hat{\phi}(\vec{x}), \hat{\phi}^+(\vec{y})\right] = \delta^3(\vec{x}-\vec{y})$ 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

$$\hat{K} = \sum_k \hbar\Omega(k)\hat{c}_k^+\hat{c}_k + K_0$$

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

$$V(\vec{x}-\vec{y}) = \frac{e^2}{|\vec{x}-\vec{y}|} \tag{19.-18}$$

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

$$\hat{K} = \hat{H} - \mu\hat{N} = \sum_k \varepsilon(k)\left(\hat{a}_{k\uparrow}^+\hat{a}_{k\uparrow} + \hat{a}_{k\downarrow}^+\hat{a}_{k\downarrow}\right) + \sum_k \left[\Delta\hat{a}_{k\uparrow}^+\hat{a}_{-k\downarrow} + \Delta^*\hat{a}_{-k\downarrow}^+\hat{a}_{k\uparrow}\right]$$

where $\hat{a}_{k\uparrow,\downarrow}^+$ are creation operators of an electron of spin up or down and momentum $\vec{k}$ and

$$\Delta = -\frac{g}{V}\sum_{k'}{}' \langle GS|\, \hat{a}_{-k\downarrow}\hat{a}_{k\uparrow}\, |GS\rangle$$

$|GS\rangle$ is the ground state of $\hat{K}$ and $\sum_{k'}{}'$ is a sum over states with

$$0 \leq \varepsilon(k') \leq \hbar\omega_m \text{ and } \varepsilon(k') = \varepsilon(k) - \mu = \frac{\hbar^2 k^2}{2m} - \mu$$

(a) Diagonalize $\hat{K}$ by a Bogoliubov transformation, i.e., introduce new operators

$$\hat{A}_k = u_k \hat{a}_{k\uparrow} - v_k \hat{a}^+_{-k\downarrow} \ , \ \hat{B}_k = v_k \hat{a}_{k\uparrow} + u_k \hat{a}^+_{-k\downarrow}$$

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

$$u_k = \left[\frac{1}{2}(1+\alpha_k)\right]^{1/2} \quad , \quad v_k = -\left[\frac{1}{2}(1-\alpha_k)\right]^{1/2}$$

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

$$\hat{K} = \sum_k E(k)\left[hatA_k^+ \hat{A}_k + \hat{B}_k^+ \hat{B}_k\right] + K_0$$

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

$$N(\varepsilon)\, d\varepsilon = \frac{d^3 k}{(2\pi)^3}$$

and assume that $N(\varepsilon) \approx N(0)$.

(c) Obtain the *distribution function* $\langle GS|\,\hat{a}^+_{k\uparrow}\hat{a}_{k\uparrow}\,|GS\rangle$

(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: $\hat{u}_n \to \hat{u}_k$, $\hat{p}_n \to \hat{p}_k$ and then introduce the creation and annihilation operators of *phonons* $\hat{a}_k^+$ and $\hat{a}_k$ by the following formula:

$$\hat{u}_k = \sqrt{\frac{\hbar}{2m\omega(k)}}(\hat{a}_k + \hat{a}_k^+) \quad , \quad \hat{p}_k = -i\sqrt{\frac{\hbar m\omega(k)}{2}}(\hat{a}_k - \hat{a}_k^+)$$

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 $t_n = t =$ constant, diagonalize the electron Hamiltonian by Fourier transform $\hat{\psi}_n \to \hat{\psi}_k$, 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 $\vec{r}$: $\vec{j}_e(\vec{r}) = \frac{e}{2m} \sum_\ell [\vec{p}_\ell \delta(\vec{r} - \vec{r}_\ell) + \delta(\vec{r} - \vec{r}_\ell)\vec{p}_\ell]$

(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

20.8 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) $\sum_s u(p.s)\bar{u}(p,s) = \not{p} + m$

(e) $\sum_s v(p.s)\bar{v}(p,s) = \not{p} - m$

(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., $\left(i\gamma^\mu \partial'_\mu - m\right)\psi'(x') = 0$, 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

$$\psi_R(x) = \frac{1}{2}(1+\gamma_5)\psi(x) \quad , \quad \psi_L(x) = \frac{1}{2}(1-\gamma_5)\psi(x)$$

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

$$\gamma^0 = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix} \quad , \quad \boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix}$$

we have

$$\psi = \begin{pmatrix} \phi_R \\ \phi_L \end{pmatrix} e^{-ip\cdot x}$$

i.e., that the lower(upper) two components of ψ_R (ψ_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 $\sigma^{\mu\nu} = \frac{i}{2}\left[\gamma^\mu, \gamma^\nu\right]$ and the field strength $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$.

(b) Show that the dependence in the magnetic field $\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$ in the spin-dependent 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 $-\boldsymbol{\nabla}^2/2m$ ($\boldsymbol{\Sigma} = \gamma_5\gamma^0\boldsymbol{\gamma}$ is the spin matrix). Determine the value of the gyromagnetic ration g for the electron.

20.8.7 Dirac → Schrodinger

Reduce tyhe Dirac equation $(i\partial\!\!\!/ - eA\!\!\!/ - m)\psi = 0$ for the Hydrogen atom ($A^0 = -Ze/4\pi r$, $\boldsymbol{A} = 0$) to the standard Schrodinger equation

$$i\frac{\partial}{\partial t}\Psi(t, boldsymbolx) = \left(-\frac{\boldsymbol{\nabla}^2}{2m} + eA^0\right)\Psi(t, boldsymbolx)$$

in the non-relativistic limit, where $|\boldsymbol{p}|$, $A^0 \ll m$. **HINT**: You may start from the reduced form of the Dirac equation in Problem 20.6(a). Extract the leading time dependence by writing $\psi(x) = \Psi(t, \boldsymbol{x})e^{-imt}$.

20.8.8 Positive and Negative Energy Solutions

Positive energy solutions of the Dirac equation correspond to the 4-vector current $\boldsymbol{J}^\mu = 2\boldsymbol{p}^\mu = 2(E, \vec{p})$, $E > 0$. Show that the negative energy solutions correspond to the current $\boldsymbol{J}^\mu = -2(E, \vec{p}) = -2(|E|, -\vec{p}) = -2\boldsymbol{p}^\mu$, $E < 0$.

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 $\boldsymbol{u}_A$ and $\boldsymbol{u}_B$ are two-component spinors. Show that in the non-relativistic limit $\boldsymbol{u}_B \sim \beta = v/c$.

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: $p^\mu \to p^\mu - eA^\mu$.

20.8.12 Properties of γ_5

Show that:

(a) $\bar{\Psi}\gamma_5\Psi$ 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 $\hat{\boldsymbol{L}}$ 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:

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \;\;,\;\; \{\alpha_i, \beta\} = 0 \text{ with } \beta^2 = 1$$

(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 2×2 β 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.