Quantum Mechanics

Mathematical Structure 
and 
Physical Structure

Problems and Solutions

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Chapter 3

Formulation of Wave Mechanics - Part 2

3.11 Solutions

3.11.1 Free Particle in One-Dimension - Wave Functions

(a) \[ \tilde{\psi}(p, 0) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} e^{i\frac{px}{\hbar}} \psi(x, 0) \, dx \]
\[ = \frac{N}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} e^{i\frac{(x-p_0)x}{\hbar}} e^{-\frac{(x-x_0)^2}{4\sigma^2}} \, dx \]
\[ = \frac{N}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} e^{-\left[ \frac{x^2}{4\sigma^2} - \frac{x x_0}{2\sigma^2} + \frac{x_0^2}{2\sigma^2} + \frac{(p-p_0)x}{\hbar} \right]} \]
\[ = \frac{N}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} e^{-\left[ \frac{x^2}{4\sigma^2} - \frac{x_0^2}{2\sigma^2} - (\frac{p-p_0}{\hbar})x \right]} \]
\[ = \frac{N}{\sqrt{2\pi \hbar}} e^{\frac{x_0^2}{4\sigma^2}} e^{-\left[ \frac{x_0^2}{2\sigma^2} - \frac{(p-p_0)^2}{\hbar^2} \right]} \int_{-\infty}^{\infty} e^{-\left( \frac{y}{2\sigma} - \frac{p}{2\sigma\hbar} \right)^2} \frac{1}{\sqrt{\pi}} \]
\[ = N \sigma \sqrt{\frac{2}{\pi \hbar}} e^{-\frac{(p-p_0)^2}{2m \hbar} \frac{2}{\sigma^2}} e^{-\frac{(p-p_0)x_0}{\hbar}} \]

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

We have
\[ i\hbar \frac{\partial \tilde{\psi}(p, t)}{\partial t} = H \tilde{\psi}(p, t) = E_p \tilde{\psi}(p, t) = \frac{p^2}{2m} \tilde{\psi}(p, t) \]
since $\tilde{\psi}(p, t)$ is an eigenfunction of $H$ (only 1 $p$ value). This implies that

$$\tilde{\psi}(p, t) = \tilde{\psi}(p, 0)e^{-iE_p t/\hbar} = \tilde{\psi}(p, 0)e^{-ip^2 t/2m \hbar}$$

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

$$\psi(x, t) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \tilde{\psi}(p, t) dp$$

$$= \frac{1}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \frac{N\sigma}{\sqrt{\hbar}} e^{-\frac{ipx_0^2}{\hbar^2}} e^{-\frac{(p-p_0)x_0}{\hbar}} e^{-ip^2 t/2m \hbar} dp$$

$$= \frac{N\sigma}{\sqrt{\pi \hbar}} \int_{-\infty}^{\infty} e^{ipx_0/\hbar} e^{i\frac{p^2\sigma^2}{\hbar^2}} \int_{-\infty}^{\infty} e^{\frac{2ipx}{\hbar} \frac{\sigma^2}{2} + it} e^{ipx_0/\hbar} e^{\frac{p^2\sigma^2}{\hbar^2}} dp$$

$$= \frac{N\sigma}{\sqrt{\pi \hbar}} e^{ipx_0/\hbar} e^{\frac{p^2\sigma^2}{\hbar^2}} \int_{-\infty}^{\infty} e^{-\frac{-(\alpha \beta)^2}{4}} e^{\frac{\beta^2}{4}} dp$$

where

$$\alpha^2 = \frac{\sigma^2}{\hbar^2} + \frac{it}{2m \hbar}$$

and

$$-2\alpha \beta = \frac{i}{\hbar} \frac{x}{\hbar} - i \frac{x_0}{\hbar} + \frac{2p_0 \sigma^2}{\hbar^2}$$

Therefore, letting $y = \alpha p - \beta$ and $dy = \alpha dp$ we get

$$\psi(x, t) = \frac{N\sigma}{\sqrt{\pi \hbar}} e^{ipx_0/\hbar} e^{i\frac{p^2\sigma^2}{\hbar^2}} \frac{1}{\alpha} \int_{-\infty}^{\infty} e^{-y^2} dy$$

$$= \frac{N\sigma}{\sqrt{\pi \hbar}} e^{ipx_0/\hbar} e^{i\frac{p^2\sigma^2}{\hbar^2}} \frac{1}{\alpha} \int_{-\infty}^{\infty} e^{-y^2} \sqrt{\sigma^2 + \frac{it \hbar}{2m}} e^{-\frac{(x-x_0-2ip_0p_0^2/\hbar)^2}{4(\sigma^2 + \frac{it \hbar}{2m})}}$$

where we have used

$$\int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\pi}$$

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

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

increases with time.

The important terms are

$$\frac{1}{\sqrt{\sigma^2 + \frac{it \hbar}{2m}}} \rightarrow \text{amplitude decreases with time}$$

and

$$e^{-\frac{(x-x_0-2ip_0p_0^2/\hbar)^2}{4(\sigma^2 + \frac{it \hbar}{2m})}} \rightarrow \text{width(spread) increases with time}$$

A sequence of pictures below illustrates what is happening:
3.11.2 Free Particle in One-Dimension - Expectation Values

For a free particle in one-dimension

\[ H = \frac{p^2}{2m} \]

(a) Show \( \langle \hat{p}_x \rangle = \langle \hat{p}_x \rangle_{t=0} \)

\[
\frac{d\langle \hat{p}_x \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{p}_x, H] \rangle = 0 \rightarrow \langle \hat{p}_x \rangle_t = \langle \hat{p}_x \rangle_0
\]

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

\[
\frac{d}{dt} \langle x \rangle = \frac{1}{i\hbar} \langle [\hat{x}, H] \rangle = \frac{1}{2im\hbar} \langle [\hat{x}, \hat{p}_x^2] \rangle = \frac{1}{m} \langle \hat{p}_x \rangle = \frac{1}{m} \langle \hat{p}_x \rangle_0
\]

Therefore

\[
\langle x \rangle_t = \frac{1}{m} \langle \hat{p}_x \rangle_0 t + \langle x \rangle_0
\]

(c) Show \( (\Delta \hat{p}_x)^2 = (\Delta \hat{p}_x)^2_{t=0} \)

\[
\frac{d}{dt} \langle \hat{p}_x^2 \rangle = \frac{1}{i\hbar} \langle [\hat{p}_x^2, H] \rangle = 0 \rightarrow \langle \hat{p}_x^2 \rangle_t = \langle \hat{p}_x^2 \rangle_0
\]

Therefore

\[
(\Delta \hat{p}_x)^2_t = \langle \hat{p}_x^2 \rangle_t - \langle \hat{p}_x \rangle_t^2 = \langle \hat{p}_x^2 \rangle_0 - \langle \hat{p}_x \rangle_0^2 = (\Delta \hat{p}_x)^2_0
\]

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

\[
\frac{d}{dt} \langle x^2 \rangle
\]

To solve the resulting differential equation, one needs to know the time dependence of \( \langle \hat{x} \hat{p}_x + \hat{p}_x x \rangle \). Find this by considering

\[
\frac{d}{dt} \langle \hat{x} \hat{p}_x + \hat{p}_x x \rangle
\]
We have

\[ \frac{d}{dt} (\Delta x)^2 = \frac{d}{dt} (x^2) + \left( \frac{d}{dt} \langle x \rangle \right)^2 \]

Now

\[
\begin{align*}
\frac{d}{dt} \langle x^2 \rangle &= \frac{1}{i \hbar} \langle [x^2, H] \rangle = \frac{1}{2i \hbar m} \langle [x^2, p_x^2] \rangle \\
&= \frac{1}{2i \hbar m} \langle x^2 p_x^2 - p_x^2 x^2 \rangle = \frac{1}{2i \hbar m} \langle x(p_x x + i\hbar)p_x - p_x^2 x^2 \rangle \\
&= \frac{1}{2i \hbar m} \langle x p_x x p_x + i\hbar x p_x - p_x^2 x^2 \rangle \\
&= \frac{1}{2i \hbar m} \langle (p_x x + i\hbar)(p_x x + i\hbar) + i\hbar x p_x - p_x^2 x^2 \rangle \\
&= \frac{1}{2i \hbar m} \langle p_x x + 2i\hbar p_x x - \hbar^2 + i\hbar x p_x - p_x^2 x^2 \rangle \\
&= \frac{1}{2i \hbar m} \langle p_x x + i\hbar x + 2i\hbar p_x x - \hbar^2 + i\hbar x p_x - p_x^2 x^2 \rangle \\
&= \frac{1}{2i \hbar m} \langle 3i\hbar p_x x - \hbar^2 + i\hbar x p_x \rangle \\
&= \frac{1}{2i \hbar m} \langle 2i\hbar x p_x + i\hbar (xp_x - i\hbar) - \hbar^2 + i\hbar x p_x \rangle \\
&= \frac{1}{m} \langle p_x x + xp_x \rangle
\end{align*}
\]

We then get

\[
\begin{align*}
\frac{d}{dt} \langle p_x x + xp_x \rangle &= \frac{1}{i \hbar} \langle [(p_x x + xp_x), H] \rangle = \frac{1}{2i \hbar m} \langle [p_x x, p_x^2] + [xp_x, p_x^2] \rangle \\
&= \frac{1}{2i \hbar m} \langle p_x x p_x^2 - p_x^3 x + xp_x^3 - p_x^2 xp_x \rangle \\
&= \frac{1}{2i \hbar m} \langle p_x (p_x x + i\hbar)p_x - p_x^3 x + xp_x^3 - p_x p_x^2 x + i hp_x^2 \rangle \\
&= \frac{1}{2i \hbar m} \langle p_x^2 (p_x x + i\hbar) + 2i\hbar p_x^2 - p_x^3 x + xp_x^3 - (xp_x - i\hbar)p_x \rangle \\
&= \frac{1}{2i \hbar m} \langle 4i\hbar p_x^2 \rangle = \frac{2}{m} \langle p_x^2 \rangle = \frac{2}{m} \langle p_x^2 \rangle_0 \\
\end{align*}
\]

where we have used the result from part (c). Therefore,

\[ \langle p_x x + xp_x \rangle_t = \frac{2}{m} \langle p_x^2 \rangle_0 t + \langle p_x x + xp_x \rangle_0 \]

and we get

\[ \frac{d}{dt} \langle x^2 \rangle = \frac{2}{m^2} \langle p_x^2 \rangle_0 t + \frac{1}{m} \langle p_x x + xp_x \rangle_0 \]
which implies that
\[ \langle x^2 \rangle_t = \frac{1}{m^2} \langle p_x^2 \rangle_0 t^2 + \frac{1}{m} \langle p_x x + x p_x \rangle_0 t + \langle x^2 \rangle_0 \]

Therefore,
\[
\frac{d}{dt} (\Delta x)^2 = \frac{d}{dt} \langle x^2 \rangle - \frac{d}{dt} \langle x \rangle^2 \\
= \frac{2}{m^2} \langle p_x^2 \rangle_0 t + \frac{1}{m} \langle p_x x + x p_x \rangle_0 - \frac{d}{dt} \left( \frac{1}{m} \langle p_x \rangle_0 t + \langle x \rangle_0 \right)^2 \\
= \frac{1}{m} \langle p_x x + x p_x \rangle_0 - \frac{2}{m} \langle p_x \rangle_0 \langle x \rangle_0 
\]

### 3.1.1.3 Time Dependence

Given
\[ H \psi = i \hbar \frac{\partial \psi}{\partial t} \]
with
\[ H = \vec{p} \cdot \vec{p} + V(\vec{x}) \]

(a) Show that \( \frac{d}{dt} \langle \psi(t) | \psi(t) \rangle = 0 \)
\[
\frac{d}{dt} \langle \psi(t) | \psi(t) \rangle = \frac{d}{dt} \int \psi^*(t) \psi(t) \, dx \\
= \int \frac{d\psi^*}{dt} \psi \, dx + \int \psi^* \frac{d\psi}{dt} \, dx \\
= - \frac{1}{i\hbar} \int (H\psi)^* \psi \, dx + \frac{1}{i\hbar} \int \psi^* H \psi \, dx \\
= - \frac{1}{i\hbar} \int \psi^* H \psi \, dx + \frac{1}{i\hbar} \int \psi^* H \psi \, dx = 0
\]
where we have used hermiticity in the last step.

(b) Show that \( \frac{d}{dt} \langle x \rangle = \langle \frac{p_x}{m} \rangle \)
\[
\frac{d}{dt} \langle x \rangle = \frac{1}{i\hbar} \langle [x, H] \rangle = \frac{1}{2im\hbar} \langle [x, p_x^2] \rangle \\
= \frac{1}{2im\hbar} \langle p_x \rangle = \frac{1}{m} \langle p_x \rangle
\]

(c) Show that \( \frac{d}{dt} \langle p_x \rangle = \langle -\frac{\partial V}{\partial x} \rangle \)
\[
\frac{d}{dt} \langle p_x \rangle = \frac{1}{i\hbar} \langle [p_x, H] \rangle = \frac{1}{i\hbar} \langle [p_x, V(x)] \rangle = \frac{1}{i\hbar} \left\langle [p_x, \sum_n V_n x^n] \right\rangle \\
= \frac{1}{i\hbar} \sum_n V_n \langle [p_x, x^n] \rangle = - \left\langle \sum_n V_n n x^{n-1} \right\rangle = - \left\langle \frac{\partial V}{\partial x} \right\rangle \\
\]
where we have used \([p_x, x^n] = -i\hbar n x^{n-1}.\)
(d) Find $\frac{d}{dt} \langle H \rangle$

$$\frac{d}{dt} \langle H \rangle = \frac{1}{i\hbar} \langle [H, H] \rangle = 0$$

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

Classically we have

$$\frac{d\vec{L}}{dt} = \frac{d}{dt}(\vec{x} \times \vec{p}) = \vec{v} \times \vec{p} + \vec{x} \times \frac{d\vec{p}}{dt} = \vec{x} \times \vec{F} = \tau$$

Quantum Mechanically, we have

$$\frac{d}{dt} \langle L_z \rangle = \frac{1}{i\hbar} \langle [L_z, H] \rangle = \frac{1}{i\hbar} \left\langle \left( [xp_y - yp_x, \left( \frac{p_x^2}{2m} + V(\vec{x}) \right) \right] \right\rangle$$

$$= \frac{1}{2im\hbar} [x, p_x^2]p_y - \frac{p_x}{2im\hbar} [y, p_y^2] + \frac{x}{i\hbar} [p_y, V(\vec{x})] - \frac{y}{i\hbar} [p_x, V(\vec{x})]$$

$$= \frac{1}{2i\hbar} \left( \frac{x}{m} + \frac{i\hbar}{2m} \frac{x}{m} \right) = \frac{x}{m} \frac{\hbar}{2m} + \frac{x}{i\hbar} \left( -i\hbar \frac{\partial V}{\partial x} \right) - \frac{y}{i\hbar} \left( -i\hbar \frac{\partial V}{\partial x} \right)$$

$$= yF_x - xF_y = \tau_z$$

which is the same equation!

### 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 $x$.

The mean value of $x$ is

$$\bar{x} = \frac{\int_0^\infty xp(x)dx}{\int_0^\infty p(x)dx} = \frac{\int_0^\infty x^2e^{-x/\lambda}dx}{\int_0^\infty xe^{-x/\lambda}dx} = \lambda \frac{\Gamma(3)}{\Gamma(2)} = 2\lambda$$

The standard deviation is defined by

$$\sigma^2 = \bar{x}^2 - (\bar{x})^2$$

Now

$$\frac{\bar{x}^2}{\bar{x}} = \frac{\int_0^\infty x^2p(x)dx}{\int_0^\infty p(x)dx} = \frac{\int_0^\infty x^3e^{-x/\lambda}dx}{\int_0^\infty xe^{-x/\lambda}dx} = \lambda \frac{\Gamma(4)}{\Gamma(2)} = 6\lambda^2$$

Therefore,

$$\sigma^2 = 6\lambda^2 - 4\lambda^2 = 2\lambda^2 \to \sigma = \sqrt{2\lambda}$$
The probability density is an extremum when

\[ p'(x) = e^{-x/\lambda} - \frac{x}{\lambda} e^{-x/\lambda} = 0 \quad (3.1) \]

at \( x = \lambda \) or as \( x \to \infty \). Note that \( \lambda > 0 \) if \( p(x) \) is to be finite in \( 0 < x < \infty \).

Since

\[ p''(x) = -\frac{2}{\lambda} e^{-x/\lambda} + \frac{x}{\lambda^2} e^{-x/\lambda} \]

We have

\[ p''(\lambda) = -\frac{1}{\lambda} e^{-1} < 0 \quad , \quad \lim_{x \to \infty} p''(x) = 0 \]

the probability density is a maximum at \( x = \lambda \). Hence, the most probable value of \( x \) is \( \lambda \).

### 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 \(-a/2 \leq x \leq a/2\), so that its wave function is

\[ \psi(x) = \begin{cases} \frac{1}{\sqrt{a}} e^{i p_0 x / \hbar} & -a/2 \leq x \leq a/2 \\ 0 & \text{otherwise} \end{cases} \]

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

The normalization integral is

\[ \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-a/2}^{a/2} |A|^2 dx = a |A|^2 = 1 \rightarrow A = e^{i \phi} \]

where the overall phase \( \phi \) is arbitrary. We set \( \phi = 0 \) from now on. Therefore we have

\[ \psi(x) = \begin{cases} \frac{1}{\sqrt{a}} e^{i p_0 x / \hbar} & -a/2 \leq x \leq a/2 \\ 0 & \text{otherwise} \end{cases} \]

The various sketches are shown below:
Note that the probability density in position space does not depend on the momentum $p_0$.

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

$$
\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)e^{-ipx/\hbar}dx = \frac{1}{\sqrt{2\pi\hbar a}} \int_{-a/2}^{a/2} \psi(x)e^{-i(p-p_0)x/\hbar}dx
$$

$$
= \frac{1}{\sqrt{2\pi\hbar a}} - \frac{\hbar}{i(p-p_0)} \bigg|_{-a/2}^{a/2} = 2\frac{1}{\sqrt{2\pi\hbar a}} \sin \left( \frac{(p-p_0)a}{\hbar} \right)
$$

Thus,

$$
\tilde{\phi}(p) = \sqrt{\frac{a}{2\pi\hbar}} \text{Sinc} \left( \frac{(p-p_0)a}{2\hbar} \right)
$$
where

\[ Sinc(x) = \frac{\sin(x)}{x} \]

A sketch is shown below:

![Figure 3.4: \( \tilde{\phi}(p) \)](image)

Note the phase-shift duality. The normalization of the momentum space wave function is given by

\[
\int_{-\infty}^{\infty} |\tilde{\phi}(p)|^2 dp = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{a}{\hbar} Sinc^2 \left( \frac{(p-p_0)a}{2\hbar} \right) \, dy = 1
\]

where we have substituted \( y = pa/\hbar \) and the result

\[
\int_{-\infty}^{\infty} Sinc^2 \left( \frac{(y-y_0)}{2} \right) \, dy = 2\pi
\]

So, as expected, given a normalized \( \psi(x) \), \( \tilde{\phi}(p) \) will also be normalized. This is just a theorem from Fourier transforms.

(c) Find the uncertainties \( \Delta x \) and \( \Delta p \) at this time. How close is this to the minimum uncertainty wave function.

We can estimate \( \Delta x \) and \( \Delta p \) by eye looking at the probability distributions \( |\psi(x)|^2 \) and \( |\phi(p)|^2 \).

Clearly, \( \Delta x \approx a \). If we take \( \Delta p \) to be the width indicated in the last figure, i.e., \( \Delta p \approx 4\pi\hbar/a \), then we get

\[ \Delta x \Delta p \approx 4\pi\hbar \]

which is not quite minimum uncertainty. Formally calculating, we have

\[ \Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \]
with \( \langle x \rangle = 0 \) by inspection and
\[
\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 \, dx = \int_{-a/2}^{a/2} \frac{x^2}{a} \, dx = \frac{a^2}{12} \rightarrow \Delta x = \frac{a}{\sqrt{12}}
\]
We also have
\[
\Delta x = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}
\]
with \( \langle p \rangle = p_0 \) by inspection and
\[
\langle p^2 \rangle = \int_{-\infty}^{\infty} p^2 |\tilde{\phi}(p)|^2 \, dp = \int_{-\infty}^{\infty} p^2 \frac{dp}{\hbar} \frac{\sin^2 (p - p_0)a/2}{(p - p_0)^2} = \infty !!!!
\]
This implies that \( \Delta p = \infty !!!! \). The formal variance diverges!. What happened? It is because of the discontinuity in \( |\psi(x)|^2 \), which via Fourier transforms then requires all values of \( p \) to be included. This is not physical!!

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.

For simplicity, we will consider only motion in the \( x - y \) plane (\( y \) vertical and \( x \) horizontal). If there was no uncertainty principle, then a dart released from a height \( h \) above the point \( x = 0 \) would strike the point \( x = 0 \) since we can set both \( x(0) = 0 \) and \( v_x(0) = 0 \) initially. Quantum mechanics does not let us do this, however. Assume that \( y(0) = h = 1 \) m and \( v_y(0) = 0 \) for the vertical motion.

Any uncertainty principle effects will be negligible in the vertical direction.

We also assume that \( x(0) = \Delta x \) and \( v_x(0) = p_x(0)/m = p_x(0) = \Delta p \), where \( \Delta x \Delta p \approx \hbar \). We then have the following equations of motion:

\[
y(t) = y(0) + v_y(0)t - \frac{1}{2}gt^2 = h - \frac{1}{2}gt^2
\]
\[
x(t) = x(0) + v_x(0)t = \Delta x + \Delta p t \rightarrow t = \frac{x - \Delta x}{\Delta p}
\]

We then have
\[
y = h - \frac{1}{2}g \left( \frac{x - \Delta x}{\Delta p} \right)^2
\]

We are interested in finding the minimum value of \( x \) when \( y = 0 \) (hits the ground). Substituting \( y = 0, h = 1 \) m, \( g = 10 \) m/sec\(^2\), \( \Delta p = \hbar/\Delta x \) and solving for \( x \) we get
\[
x = \Delta x + \frac{0.45h}{\Delta x} \tag{3.2}
\]
We find the minimum by computing
\[ \frac{\partial x}{\partial \Delta x} = 0 = 1 - \frac{0.45\hbar}{(\Delta x)^2} \rightarrow \Delta x = \sqrt{0.45\hbar} \]

Therefore, the minimum \( x \) consistent with quantum mechanics is
\[ x_{\text{min}} = 2\sqrt{0.45\hbar} \approx 10^{-17} \text{m} \]

This is a very small distance! An atomic nucleus has a diameter of \( 10^{-15} \text{ m} \).

**3.11.7 Find the Potential and the Energy**

Suppose that the wave function of a (spinless) particle of mass \( m \) is
\[ \psi(r, \theta, \phi) = A e^{-\alpha r} - e^{-\beta r} \]

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

Write the wave function as
\[ \psi(r, \theta, \phi) = A \frac{e^{-\alpha r} - e^{-\beta r}}{r} = \frac{u(r)}{r} \]

Since \( \psi \) depends only on \( r \), we have \( \ell = m = 0 \), and the Schrodinger equation in spherical coordinates is
\[ -\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + (V(r) - E) u = 0 \rightarrow V(r) - E = \frac{\hbar^2}{2m} \frac{1}{u} \frac{d^2 u}{dr^2} \]

Differentiate \( u(r) = A(e^{-\alpha r} - e^{-\beta r}) \):
\[ \frac{du}{dr} = A(-\alpha e^{-\alpha r} + \beta e^{-\beta r}) \]
\[ \frac{d^2 u}{dr^2} = A(\alpha^2 e^{-\alpha r} - \beta^2 e^{-\beta r}) \]

This gives
\[ V(r) - E = \frac{\hbar^2}{2m} \frac{\alpha^2 e^{-\alpha r} - \beta^2 e^{-\beta r}}{e^{-\alpha r} - e^{-\beta r}} \]

Since the potential must vanish at \( r \to \infty \), we get
\[ E = -\lim_{r \to \infty} \frac{\hbar^2}{2m} \frac{\alpha^2 e^{-\alpha r} - \beta^2 e^{-\beta r}}{e^{-\alpha r} - e^{-\beta r}} = -\frac{\hbar^2 \alpha^2}{2m} \]

and the potential is
\[ V(r) = \frac{\hbar^2}{2m} \left( \frac{\alpha^2 e^{-\alpha r} - \beta^2 e^{-\beta r}}{e^{-\alpha r} - e^{-\beta r}} - \alpha^2 \right) \]
For small $r$:  
\[ V(r) \approx -\frac{\hbar^2}{2m} \frac{(\alpha^2 - \beta^2)e^{-\beta r}}{(\beta - \alpha)r} = -\frac{\hbar^2(\alpha + \beta)e^{-\beta r}}{2mr} \]

This is a screened Coulomb potential.

The same procedure to find $V$, $E$ also works if $\psi$ has an angular dependence, by including the centrifugal barrier term $\ell(\ell + 1)\hbar^2/2mr^2$ in the radial Schrödinger equation.

### 3.11.8 Harmonic Oscillator wave Function

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

![Figure 3.5: A Wave Function](image)

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

The plot shows one node which implies that it is the first excited state. Alternatively, the Schrödinger equation  
\[-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \quad , \quad V(x) = \frac{1}{2}m\omega^2x^2\]

gives  
\[-\frac{\hbar^2}{2m} \frac{d}{dx} \left( Ax e^{(-x^2/x_0^2)} - \frac{2x^2}{x_0^2} Ax e^{(-x^2/x_0^2)} \right) + V(x)\psi = E\psi \]
\[-\frac{\hbar^2}{2m} \left( -\frac{6}{x_0^2} + \frac{4x^2}{x_0^4} \right) \psi + \frac{1}{2}m\omega^2x^2\psi = E\psi \]

Taking $\lim_{x \to \infty}$ says that we must have  
\[ \frac{4\hbar^2x^2}{2mx_0^2} = \frac{1}{2}m\omega^2 \rightarrow x_0^2 = \frac{2\hbar}{m\omega} \]
We then have

\[ E = -\frac{\hbar^2}{2m} \left( -\frac{6}{x_0^2} \right) = \frac{3}{2} \hbar \omega \]

which corresponds to the first excited state energy.

(b) Is this an eigenstate of parity?

We have using the parity operator \( \hat{P} \)

\[ \hat{P} \psi(x) = \hat{P}(Axe^{-x^2/x_0^2}) = A(-x)e^{(-x)^2/x_0^2} = -Axe^{(-x^2/x_0^2)} = -\psi(x) \]

Therefore, it is an eigenstate of \( \hat{P} \) with eigenvalue \(-1\).

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

We have

\[ 1 = \int_{-\infty}^{\infty} |\psi|^2 dx = A^2 \int_{-\infty}^{\infty} x^2 e^{(-2x^2/x_0^2)} dx \]

Changing variables with \( y = \sqrt{2}x/x_0 \), we get

\[ 1 = A^2 \frac{x_0^3}{2\sqrt{2}} \int_{-\infty}^{\infty} y^2 e^{-y^2} dy \]

Using

\[ \int_{-\infty}^{\infty} y^2 e^{-y^2} dy = \frac{\sqrt{\pi}}{2} \]

we get

\[ 1 = A^2 \frac{x_0^3}{2\sqrt{2}} \frac{\sqrt{\pi}}{2} \rightarrow A^2 = \sqrt{\frac{2}{\pi}} \frac{4}{x_0^3} \]

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 \( \omega \) 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

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

For a general wave packet we have

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)e^{ikx}dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k; x)dk$$

i.e., an infinite superposition of planes waves (free-space stationary states) with arbitrary coefficients, $b(k)$. Including the coefficients $b(k)$ given by the Fourier transform relation

$$b(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x, 0)e^{-ikx}dx$$

in the stationary state $\phi(k; x)$ gives the last integral above.

But we know the time dependence of the stationary states $\phi(k; x)$ from the time-dependent Schrödinger equation

$$i\hbar \frac{d}{dt}\phi(k; x, t) = \hat{H}\phi(k; x, t)$$

with $\hat{H} = \hat{p}^2/2m$ for free space. This implies that

$$\phi(k; x, t) = \phi(k; x, 0)e^{-i\omega t}$$

where $\omega = \omega(k)$ is given by

$$E = \hbar \omega(k) = \frac{\hbar^2k^2}{2m}$$

Since we know the time dependence of the individual terms in the integral, we just integrate to get the overall time dependence which is then not stationary

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k; x, t)dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)e^{i(kx-\omega(k)t)}dk$$

We then have

$$b(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x', 0)e^{-ikx'}dx'$$

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k; x, t)dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left( \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x', 0)e^{-ikx'}dx' \right) e^{i(kx-\omega(k)t)}dk$$

$$= \int_{-\infty}^{\infty} dx' \psi(x', 0) \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-i(\omega(k)t-k(x-x'))}$$

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We then define
\[ K(x, x', t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-i(\omega t - k(x-x'))} \]
as the Free Space Propagator. We can evaluate the propagator by completing the square with \( \omega = \hbar k^2/2m \). Using
\[ A^2k^2 + 2ABk(x-x') + B^2(x-x')^2 = \frac{\hbar t}{2m} k^2 - k(x-x') + B^2(x-x')^2 \]
we require that
\[ A^2 = \frac{\hbar t}{2m}, \quad 2AB = -1, \quad B^2 = \frac{m}{2\hbar t} \]
and the expression for \( K \) becomes
\[ K(x, x', t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-i(\sqrt{\frac{\hbar t}{2m}}k - \sqrt{\frac{m}{\hbar t}}(x-x'))^2} e^{i\frac{m}{\hbar t}k(x-x')} \]
If we let
\[ u = \sqrt{\frac{\hbar t}{2m}}k - \sqrt{\frac{m}{2\hbar t}}(x-x') \rightarrow du = \sqrt{\frac{\hbar t}{2m}} dk \]
we get
\[ K(x, x', t) = \frac{1}{2\pi} \sqrt{\frac{2m}{\hbar t}} e^{-i\frac{m}{\hbar t}(x-x')^2} \int_{-\infty}^{\infty} du e^{-iu^2} \]
\[ = \frac{1}{2\pi} \sqrt{\frac{2\pi m}{i\hbar t}} e^{-i\frac{m}{\hbar t}(x-x')^2} \]
where we have used
\[ \int_{-\infty}^{\infty} du e^{-iu^2} = \sqrt{\frac{\pi}{i}} \]
and then
\[ \psi(x, t) = \int_{-\infty}^{\infty} dx' \psi(x', 0) K(x, x', t) \]
(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.

The normalization condition is
\[ \int_{-\infty}^{\infty} |\psi(x, 0)|^2 dx = \frac{1}{\sqrt{2\pi a^2}} \int_{-\infty}^{\infty} e^{-x^2/2a^2} dx = \frac{\sqrt{2\pi a^2}}{\sqrt{2\pi a^2}} = 1 \]
(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 $1 \, \text{g}$ and width $a = 1 \, \text{cm}$. Comment.

The probability distribution looks like:

\[
|\psi(x,0)|^2 = \left(\frac{1}{\sqrt{2\pi a^2}}\right)e^{-x^2/2a^2}
\]

The width $a$ gives us an estimate of $\Delta x$ at $t = 0$. Since this is the only length in the problem, we take it as one of our characteristic lengths, $x_c$

\[
x_c \equiv a \approx \Delta x
\]

The Heisenberg uncertainty principle gives

\[
\Delta x \Delta p \geq \hbar
\]

so we take the minimum momentum uncertainty at $t = 0$ for our characteristic momentum,

\[
p_c = \Delta p_{\text{min}}(t = 0) = \frac{\hbar}{\Delta x(t = 0)} = \frac{\hbar}{x_c} = \frac{\hbar}{a}
\]

We thus have the characteristic energy

\[
E_c = \frac{p_c^2}{2m} = \frac{\hbar^2}{2ma^2}
\]

Associated with any characteristic energy is a characteristic time

\[
t_c = \frac{\hbar}{E_c} = \frac{2ma^2}{\hbar}
\]

For $m = 1 \, \text{g} \, \text{m}$, $a = 1 \, \text{cm}$, we have $t + c \approx 2 \times 10^{27} \, \text{sec}$. This is much larger than the age of the universe. Thus, we do not expect to see spreading of objects anywhere near macroscopic size!
(d) Show that the wave packet probability density remains Gaussian with the solution

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

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

Using part (a)

\[ \psi(x, t) = \int_{-\infty}^{\infty} dx' K(x, x', t) \psi(x', 0) \]

\[ = \frac{1}{(2\pi a^2)^{1/4}} \sqrt{\frac{m}{2\pi i\hbar t}} \int_{-\infty}^{\infty} dx' e^{i \frac{\hbar}{2m} (x-x')^2} e^{i k_0 x'} e^{-\frac{x'^2}{4a^2}} \]

\[ = C \int_{-\infty}^{\infty} dx' \exp \left( i \frac{m}{2\hbar t} (x^2 - 2xx' - x'^2) + ik_0 x' - \frac{x'^2}{4a^2} \right) \]

\[ = C \int_{-\infty}^{\infty} dx' \exp \left( - \left( \frac{im}{2\hbar t} + \frac{1}{4a^2} \right) x'^2 + \left( ik_0 - \frac{im}{\hbar t} x \right) x' + \frac{im}{2\hbar t} x^2 \right) \]

\[ = Ce^{\frac{im}{2\hbar t}} \int_{-\infty}^{\infty} dx' \exp \left( -i \left( \left( \frac{m}{2\hbar t} - \frac{i}{4a^2} \right) x'^2 + \left( \frac{m}{\hbar t} x - k_0 \right) x' \right) \right) \]

where

\[ C = \frac{1}{(2\pi a^2)^{1/4}} \sqrt{\frac{m}{2\pi i\hbar t}} \]

We now complete the square as before.

\[ A^2x'^2 + 2ABx' + B^2 = \left( \frac{m}{2\hbar t} - \frac{i}{4a^2} \right) x'^2 + \left( \frac{m}{\hbar t} x - k_0 \right) x' \]

We then have

\[ A^2 = \left( \frac{m}{2\hbar t} - \frac{i}{4a^2} \right) \quad , \quad 2AB = \left( \frac{m}{\hbar t} x - k_0 \right) x' \]

or

\[ A = \left( \frac{m}{2\hbar t} \left( 1 - \frac{it}{t_e} \right) \right)^{1/2} \quad , \quad B = \frac{\sqrt{m} x - \frac{k_0 \hbar t}{m}}{2\hbar t \sqrt{1 - \frac{u}{t_e}}} \]

We then have

\[ \psi(x, t) = \frac{1}{(2\pi a^2)^{1/4}} \sqrt{\frac{m}{2\pi i\hbar t}} e^{i \frac{\hbar}{2m} e^{i B^2}} \int_{-\infty}^{\infty} dx' e^{-i(Ax' + B)^2} \]

Now let \( u = Ax' + B \), \( du = Adx' \). We then have

\[ I = \frac{1}{A} \int_{-\infty}^{\infty} du e^{-iu^2} = \frac{1}{A} \sqrt{\frac{\pi}{i}} = \frac{1}{A} \sqrt{-\pi i} \]
Thus,

$$\psi(x,t) = \frac{1}{(2\pi a^2)^{1/4}} \sqrt{\frac{m}{2\pi i\hbar}} \left(1 - \frac{it}{t_c}\right)^{-1/2} \exp\left(\frac{im}{2\hbar} x + \frac{(x - \frac{\hbar k_0}{m})^2}{2m}\right)$$

Finally we get

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

with

$$a(t) = 1 + \frac{t^2}{t_c^2}$$

### 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 $\psi$). Comment on the relation of this result to the uncertainty principle.

We have

$$\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx = \frac{1}{\sqrt{4\pi \hbar a}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} dx$$

$$= \frac{1}{\sqrt{4\pi \hbar a}} \left(-\frac{\hbar}{ip}\right) \int_{-\infty}^{\infty} e^{iy} dy \text{ where } y = -\frac{ipx}{\hbar}$$

$$= \frac{1}{\sqrt{4\pi \hbar a}} \left(-\frac{\hbar}{ip}\right) \left(e^{-ip/a/\hbar} - e^{ip/a/\hbar}\right) = \frac{1}{p} \sqrt{\frac{\hbar}{\pi a}} \sin \left(\frac{pa}{\hbar}\right)$$

Therefore, $\langle p \rangle = 0$ by inspection and

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} p^2 |\tilde{\phi}(p)|^2 dp = \infty$$

The divergence is once again not physical, but is due to the artificial discontinuities in $\psi(x)$. 

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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 \( E = \frac{\hbar^2 k^2}{2m} \) to simplify the equation to

\[ (\nabla^2 + k^2) \psi(\vec{x}) = 0 \]

Show that

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

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

satisfy the equation.

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

\[ \nabla^2 \psi(\vec{x}) = \frac{d^2}{dz^2} e^{ikz} = -k^2 e^{ikz} \]

and we clearly have a solution.

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

\[ \nabla^2 \psi(\vec{x}) = \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) e^{ikr}/r = \frac{1}{r^2} \frac{d}{dr} \left( -e^{ikr} + ikr e^{ikr} \right) \]

\[ = -k^2 \psi(\vec{x}) \]

and we clearly have a solution.

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
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 $z = L \gg d$, 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

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

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

As stated, we assume that the denominators are approximately the same between the two waves. This is justified because the corrections are of order $d/L$, and we are interested in the case where $d \ll L$. We require that the numerators have the same phase, namely, $kr_+ - kr_- = 2\pi n$. We expand the LHS with respect to $d$ (using Mathematica),
Series \[\sqrt{x^2 + (y + \frac{d}{2})^2 + L^2}, \{d, 0, 1\}\]
\[
\sqrt{x^2 + y^2 + \frac{yd}{2\sqrt{x^2 + y^2}}} + O[d]^2
\]

Series \[\sqrt{x^2 + (y - \frac{d}{2})^2 + L^2}, \{d, 0, 1\}\]
\[
\sqrt{x^2 + y^2 - \frac{yd}{2\sqrt{x^2 + y^2}}} + O[d]^2
\]

Simplify[Normals[%]]
\[
\frac{dy}{\sqrt{L^2 + x^2 + y^2}}
\]

Therefore,
\[
k \frac{yd}{\sqrt{L^2 + x^2 + y^2}} = 2\pi n \rightarrow \frac{y}{\sqrt{L^2 + x^2 + y^2}} = \frac{\lambda}{d}
\]

(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.

Let us choose the unit where \(k = 1\). Then we pick \(d = 20\), \(L = 1000\). We then plot the interference pattern along the \(y\)-axis (\(x = 0\))

\[
\text{Plot} \left[ \text{Abs} \left( \frac{E_{r+}}{r_+} + \frac{E_{r-}}{r_-} \right)^2 \right. \left. \{ r_+ \rightarrow \sqrt{x^2 + (y - \frac{d}{2})^2 + L^2}, r_- \rightarrow \sqrt{x^2 + (y + \frac{d}{2})^2 + L^2} \} \right] /. \{d \rightarrow 20, L \rightarrow 1000\} /. \{x \rightarrow 0\}, \{y, -3000, 3000\}, \text{PlotPoints} \rightarrow 100]
\]

(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 \emph{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 observed 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?

For the same parameters as in (b) we have along the \( y \)-axis (\( x = 0 \)
The main difference is the absence of the interference pattern.
3.11.13 A Falling Pencil

Using the uncertainty principle estimate how long a time a pencil can be balanced on its point.

Consider the diagram below:

We have Newton’s equation of motions for the CM of the pencil:

\[ I \ddot{\theta} = mgr \sin \theta - \dot{\theta} \frac{d\dot{\theta}}{d\theta} = \frac{mgr}{I} \sin \theta \]

Integrating, we get the energy conservation equation:

\[ \frac{\dot{\theta}^2 - \dot{\theta}_0^2}{2} = -\frac{mgr}{I} (\cos \theta - \cos \theta_0) \]

We then get

\[ \frac{d\theta}{dt} = \sqrt{\dot{\theta}_0^2 - \frac{mgr}{I} (\cos \theta - \cos \theta_0)} \]

which implies (integrating)

\[ t = K_1 \int_{\theta_0}^{\theta_0'} \frac{d\theta}{\sqrt{K_2 - \cos \theta}} \]

where

\[ K_1 = \sqrt{\frac{I}{2mgr}} \quad , \quad K_2 = \frac{I\dot{\theta}_0^2 + 2mgr \cos \theta_0}{2mgr} \]

Now we assume that \( \theta_0 \approx (\Delta \theta)_0, \dot{\theta}_0 \approx (\Delta \dot{\theta})_0 \) which says that the best possible initial conditions are given by the uncertainties. If we are trying to balance the pencil for the longest time, then \( \theta_0 \) and \( \dot{\theta}_0 \) must be as small as possible. Therefore we have

\[ K_2 \approx 1 + \epsilon \quad , \quad \epsilon \ll 1 \]
Therefore, small $\theta$ values will dominate the integral, i.e., the pencil spends most of its time at small $\theta$. You can see that this is true by trying an experiment!

Therefore we can write $\cos \theta \approx 1 - \theta^2 / 2$ which gives

$$t = K_1 \int_{\theta_0}^{\theta_f} \frac{d\theta}{\sqrt{K_3 + \frac{\alpha \theta^2}{2}}}$$

where $K_3 = K_2 - 1 = \epsilon$. Now let

$$\theta = \sqrt{2K_3} \tan \phi \rightarrow d\theta = \sqrt{2K_3} \sec^2 \phi$$

We then have

$$t = K_1 \int_{\phi_0}^{\phi_f} \sec \phi d\phi$$

where

$$\phi_0 = \tan^{-1} \left( \frac{\theta_0}{\sqrt{2K_3}} \right), \quad \phi_1 = \tan^{-1} \left( \frac{\theta_f}{\sqrt{2K_3}} \right)$$

Now

$$\int \sec \phi d\phi = \ln(\sec \phi + \tan \phi)$$

Therefore, we get

$$t = \sqrt{2}K_1 \ln \frac{\sec \phi_f + \tan \phi_f}{\sec \phi_0 + \tan \phi_0}$$

The uncertainty principle says (at best) that initially

$$(\Delta x_0)(\delta p_x)_0 = \hbar \rightarrow (r(\Delta \theta)_0)(mr(\delta \dot{\theta})_0) = \hbar = m\dot{r}\theta_0 \dot{\theta}_0$$

which implies that

$$\dot{\theta}_0 = \frac{\hbar}{m r^2 \theta_0}$$

Therefore,

$$K_2 \approx 1 + \frac{\theta_0^2}{2} + \alpha \frac{\hbar^2}{\theta_0^2}$$

where

$$\alpha = \frac{I}{2m^3gr^3} \approx 0.005 \text{ for a typical pencil}$$

Thus,

$$K_3 = \epsilon = \frac{\theta_0^2}{2} + \alpha \frac{\hbar^2}{\theta_0^2}$$

and

$$\phi_0 = \tan^{-1} \frac{\theta_0}{\sqrt{2K_3}} \rightarrow \tan \phi_0 \approx 1 \approx \sec \phi_0$$

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Using $\theta_f = \pi/2$ (pencil on floor), we have
\[
\frac{\theta_f}{\sqrt{2K_3}} \gg 1 \rightarrow \sec \phi_f \approx \tan \phi_f \approx \frac{\pi}{2\sqrt{2K_3}}
\]
Therefore,
\[
t \approx \sqrt{2K_1 \ln \frac{\pi}{2\sqrt{2K_3}}}
\]
where
\[
K_1 = \sqrt{\frac{I}{2mg}} \approx 0.1 \text{ for a typical pencil}
\]
Now, if we want maximum time (upright) we need to minimize $K_3$. Thus we have
\[
\frac{\partial K_3}{\partial \theta_0} = -\theta_0 - \frac{2\alpha \hbar^2}{\theta_0^3}
\]
We get
\[
\theta_0 \approx (2\alpha)^{1/4} \sqrt{\hbar} \approx \frac{1}{3} \sqrt{\hbar} \rightarrow K_3 \approx \frac{\hbar}{4}
\]
Finally, we have
\[
t_{\text{max}} \approx \frac{\sqrt{2}}{2} \frac{1}{10} (-\ln K_3) \approx 0.1(-\ln \hbar) \approx 0.1 \times 34 \approx 3 - 4 \text{ sec}
\]
Again, try a few experiments!
Chapter 4

The Mathematics of Quantum Physics:

Dirac Language

4.22 Problems

4.22.1 Simple Basis Vectors

Given two vectors
\[ \vec{A} = 7\hat{e}_1 + 6\hat{e}_2, \quad \vec{B} = -2\hat{e}_1 + 16\hat{e}_2 \]
written in the \{\hat{e}_1, \hat{e}_2\} basis set and given another basis set
\[ \hat{e}_q = \frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2, \quad \hat{e}_p = -\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2 \]

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

\[ \hat{e}_q \cdot \hat{e}_p = \left( \frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right) \cdot \left( -\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2 \right) = \frac{1}{2} \left( -\frac{\sqrt{3}}{2} \right) + \frac{\sqrt{3}}{2} \frac{1}{2} = 0 \]
so they are orthogonal.

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

\[ \begin{align*}
A_q &= \hat{e}_q \cdot \vec{A} = \left( \frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right) \cdot (7\hat{e}_1 + 6\hat{e}_2) = \frac{7}{2} + 3\sqrt{3} \\
A_p &= \hat{e}_p \cdot \vec{A} = \left( -\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2 \right) \cdot (7\hat{e}_1 + 6\hat{e}_2) = 3 - \frac{7\sqrt{3}}{2} \\
B_q &= \hat{e}_q \cdot \vec{B} = \left( \frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right) \cdot (-2\hat{e}_1 + 16\hat{e}_2) = 1 + 8\sqrt{3} \\
B_p &= \hat{e}_p \cdot \vec{B} = \left( -\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2 \right) \cdot (-2\hat{e}_1 + 16\hat{e}_2) = \sqrt{3} + 8
\end{align*} \]
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.

We have the matrix

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

The characteristic equation is given by

\[
\det |A - \lambda I| = 0 = \begin{vmatrix} 1 - \lambda & 2 & 4 \\ 2 & 3 - \lambda & 0 \\ 5 & 0 & 3 - \lambda \end{vmatrix}
\]


\[ 0 = (1 - \lambda) (3 - \lambda) (3 - \lambda) - 20 (3 - \lambda) - 4 (3 - \lambda) \]

\[ 0 = (3 - \lambda) (\lambda^2 - 4\lambda - 24) = (3 - \lambda) (3 + \lambda) (\lambda - 7) \]

with solutions (eigenvalues)

\[ \lambda_1 = 3, \lambda_2 = -3, \lambda_3 = 7 \]

We find the eigenvectors as follows:

\[ A |1\rangle = \lambda_1 |1\rangle = 3 |1\rangle \] with \[ |1\rangle = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \]

or

\[ \begin{pmatrix} 1 & 2 & 4 \\ 2 & 3 & 0 \\ 5 & 0 & 3 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 3 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \]

which is equivalent to

\[ a + 2b + 4c = 3a \]
\[ 2a + 3b = 3b \]
\[ 5a + 3c = 3c \]

which give

\[ a = 0, b = -2c \]

Since the eigenvector must be normalized to 1 we have

\[ a = 0, b = -\frac{2}{\sqrt{5}}, c = \frac{1}{\sqrt{5}} \Rightarrow |1\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix} \]
Similarly, we find
\[
|2\rangle = \frac{1}{\sqrt{65}} \begin{pmatrix} -6 \\ 2 \\ 5 \end{pmatrix}, \quad |3\rangle = \frac{1}{\sqrt{45}} \begin{pmatrix} 4 \\ 2 \\ 5 \end{pmatrix}
\]

We then find that
\[
\langle 1 | 2 \rangle = \frac{1}{\sqrt{325}} \neq 0, \quad \langle 1 | 3 \rangle = \frac{1}{\sqrt{225}} \neq 0, \quad \langle 2 | 3 \rangle = \frac{1}{\sqrt{117}} \neq 0
\]

which is OK in this case since \( A \) is not Hermitian and therefore the eigenvectors do not need to be orthogonal.

### 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.

The eigenvalues are given by the characteristic equation
\[
\det \begin{pmatrix} 2 - \lambda & 2 & 0 \\ 1 & 2 - \lambda & 1 \\ 1 & 2 & 1 - \lambda \end{pmatrix} = 0 = (2 - \lambda)^2(1 - \lambda) + 2 - 2(2 - \lambda) - 2(1 - \lambda)
\]
\[
(2 - \lambda)((2 - \lambda)(1 - \lambda) - 2) + 2\lambda = (2 - \lambda)(\lambda - 3)\lambda + 2\lambda = -\lambda(\lambda^2 - 5\lambda + 4) = 0
\]
\[
\lambda(\lambda - 4)(\lambda - 1) = 0
\]
\[
\lambda = 0, 1, 4
\]

The eigenvectors are found by
\[
\begin{pmatrix} 2 & 2 & 0 \\ 1 & 2 & 1 \\ 1 & 2 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0 \quad \Rightarrow \quad a + 2b + c = 0 \quad \Rightarrow \quad \begin{cases} a = 1/\sqrt{3} \\ a + b = 0 \quad \Rightarrow \quad b = -a \quad \Rightarrow \quad a = 1/\sqrt{3} \end{cases}
\]
\[
|0\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}
\]

\[
\begin{pmatrix} 2 & 2 & 0 \\ 1 & 2 & 1 \\ 1 & 2 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{cases} 2a + 2b + c = b = -a/2 \quad \Rightarrow \quad a = \sqrt{2}/3 \\ a = b = -a/2 \quad \Rightarrow \quad b = -1/\sqrt{6} \end{cases}
\]
\[
|1\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}
\]

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4.22.4 Operator Matrix Representation

\[
\begin{pmatrix}
2 & 2 & 0 \\
1 & 2 & 1 \\
1 & 2 & 1
\end{pmatrix}
\begin{pmatrix}
a \\
b \\
c
\end{pmatrix} = 4
\begin{pmatrix}
a \\
b \\
c
\end{pmatrix}
\Rightarrow
\begin{align*}
a + 2b &= 4a \\
b + 2c &= 4b \\
a^2 + b^2 + c^2 &= 1
\end{align*}
\Rightarrow
\begin{align*}
b &= a \\
c &= a \\
c &= 1/\sqrt{3}
\end{align*}

\[
|4\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}
\]

Gram-Schmidt:

\[
|0'\rangle = |0\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}
\]

\[
|1'\rangle = |1\rangle - \frac{\langle 1 | 0' \rangle}{\langle 0' | 0' \rangle} |0'\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix} - \frac{2}{\sqrt{3} \sqrt{3}} \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} 4 \\ -1 \\ -5 \end{pmatrix}
\]

\[
|4'\rangle = |4\rangle - \frac{\langle 4 | 0' \rangle}{\langle 0' | 0' \rangle} |0'\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \frac{1}{\sqrt{3} \sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} 4 \\ -1 \\ -5 \end{pmatrix}
\]

\[
\frac{3}{7\sqrt{3}} \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix} \Rightarrow \frac{1}{\sqrt{14}} \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix}
\]

giving the orthonormal set of eigenvectors

\[
|0'\rangle = |0\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} , \quad |1'\rangle = \frac{1}{\sqrt{42}} \begin{pmatrix} 4 \\ -1 \\ -5 \end{pmatrix} , \quad |4'\rangle = \frac{1}{\sqrt{14}} \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix}
\]

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

\[
\hat{G} |1\rangle = 2 |1\rangle - 4 |2\rangle + 7 |3\rangle \\
\hat{G} |2\rangle = -2 |1\rangle + 3 |3\rangle \\
\hat{G} |3\rangle = 11 |1\rangle + 2 |2\rangle - 6 |3\rangle
\]

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

We have

\[
\begin{align*}
\langle 1 | \hat{G} | 1 \rangle &= 2 \langle 1 | 1 \rangle - 4 \langle 1 | 2 \rangle + 7 \langle 1 | 3 \rangle = 2 = G_{11} \\
\langle 2 | \hat{G} | 1 \rangle &= 2 \langle 2 | 1 \rangle - 4 \langle 2 | 2 \rangle + 7 \langle 2 | 3 \rangle = -4 = G_{21} \\
\langle 3 | \hat{G} | 1 \rangle &= 2 \langle 3 | 1 \rangle - 4 \langle 3 | 2 \rangle + 7 \langle 3 | 3 \rangle = 7 = G_{31} \\
\langle 1 | \hat{G} | 2 \rangle &= -2 \langle 1 | 1 \rangle + 3 \langle 1 | 3 \rangle = -2 = G_{12} \\
\langle 2 | \hat{G} | 2 \rangle &= -2 \langle 2 | 1 \rangle + 3 \langle 2 | 3 \rangle = 0 = G_{22} \\
\langle 3 | \hat{G} | 2 \rangle &= -2 \langle 3 | 1 \rangle + 3 \langle 3 | 3 \rangle = 3 = G_{32} \\
\langle 1 | \hat{G} | 3 \rangle &= 11 \langle 1 | 1 \rangle + 2 \langle 1 | 2 \rangle - 6 \langle 1 | 3 \rangle = 11 = G_{13} \\
\langle 2 | \hat{G} | 3 \rangle &= 11 \langle 2 | 1 \rangle + 2 \langle 2 | 2 \rangle - 6 \langle 2 | 3 \rangle = 2 = G_{23} \\
\langle 3 | \hat{G} | 3 \rangle &= 11 \langle 3 | 1 \rangle + 2 \langle 3 | 2 \rangle - 6 \langle 3 | 3 \rangle = -6 = G_{33}
\end{align*}
\]
so that

\[ G = \begin{pmatrix} 2 & -2 & 11 \\ -4 & 0 & 2 \\ 7 & 3 & -6 \end{pmatrix} \]

### 4.22.5 Matrix Representation and Expectation Value

If the states \{\ket{1}, \ket{2}, \ket{3}\} form an orthonormal basis and if the operator \( \hat{K} \) has the properties

\[
\hat{K} \ket{1} = 2 \ket{1} \\
\hat{K} \ket{2} = 3 \ket{2} \\
\hat{K} \ket{3} = -6 \ket{3}
\]

(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 \{\ket{1}, \ket{2}, \ket{3}\} basis.

These are eigenvectors of \( \hat{K} \) so we can immediately write

\[ \hat{K} = 2 \ket{1} \bra{1} + 3 \ket{2} \bra{2} - 6 \ket{3} \bra{3} \]

Any matrix representing an operator written in the basis of its own eigenvectors is diagonal with the eigenvalues on the diagonal. Thus

\[ \hat{K} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix} \]

(b) What is the expectation or average value of \( \hat{K} \), defined as \( \bra{\alpha} \hat{K} \ket{\alpha} \), in the state

\[ \ket{\alpha} = \frac{1}{\sqrt{83}} (-3 \ket{1} + 5 \ket{2} + 7 \ket{3}) \]

We have

\[ \ket{\alpha} = \frac{1}{\sqrt{83}} (-3 \ket{1} + 5 \ket{2} + 7 \ket{3}) \]

and

\[ \braket{\hat{K}} = \bra{\alpha} \hat{K} \ket{\alpha} = \sum_{n=1}^{3} k_n P(k_n) \]

We will evaluate this in three ways.

**Matrix Multiplication:**

\[
\braket{\hat{K}} = \bra{\alpha} \hat{K} \ket{\alpha} = \frac{1}{\sqrt{83}} (-3, 5, 7) \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix} \frac{1}{\sqrt{83}} \begin{pmatrix} -3 \\ 5 \\ 7 \end{pmatrix} = -\frac{201}{83}
\]
Bra-Kets:

\[ \langle \hat{K} \rangle = \frac{1}{\sqrt{83}} (-3 \langle 1 | + 5 \langle 2 | + 7 \langle 3 |) (2 | 1 \rangle (1 + 3 | 2 \rangle \langle 2 | - 6 | 3 \rangle \langle 3 |) \frac{1}{\sqrt{83}} (-3 | 1 \rangle + 5 | 2 \rangle + 7 | 3 \rangle) \]
\[ = \frac{1}{\sqrt{83}} (-3 (1 + 5 | 2 \rangle + 7 | 3 \rangle) (-6 | 1 \rangle + 15 | 2 \rangle - 42 | 3 \rangle) - \frac{201}{83} \]

Probabilities:

\[ \langle \hat{K} \rangle = \langle \alpha | \hat{K} | \alpha \rangle = \sum_{n=1}^{3} k_n P(k_n) = 2 |(1 | \alpha \rangle|^2 + 3 |(2 | \alpha \rangle|^2 - 6 |(3 | \alpha \rangle|^2 \]
\[ = 2 \frac{9}{83} + 3 \frac{25}{83} - 6 \frac{49}{83} = -\frac{201}{83} \]

### 4.22.6 Projection Operator Representation

Let the states \{\ket{1}, \ket{2}, \ket{3}\} 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

\[ |A \rangle = \frac{1}{\sqrt{83}} (-3 | 1 \rangle + 5 | 2 \rangle + 7 | 3 \rangle) \]

What is the result of \( \hat{P}_2 |A \rangle \)?

Since this is an orthonormal basis, we have

\[ P_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

Its eigenvalues are \( \lambda = 1, 0, 0 \) and its eigenvectors are

\[ |0 \rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |2 \rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3 \rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \]

Finally,

\[ \hat{P}_2 |A \rangle = |2 \rangle \langle 2 | A \rangle = \frac{5}{\sqrt{83}} |2 \rangle \]

We also note that

\[ \hat{P}_2^2 = (|2 \rangle \langle 2 |)(|2 \rangle \langle 2 |) = |2 \rangle \langle 2 | = \hat{P}_2 \]
\[ \hat{P}_2^2 |\lambda \rangle = P_2 |\lambda \rangle = \lambda |\lambda \rangle \]
\[ = \hat{P}_2 (\hat{P}_2 |\lambda \rangle) \]
\[ = \hat{P}_2 (\lambda |\lambda \rangle) = \lambda (\hat{P}_2 |\lambda \rangle) = \lambda^2 |\lambda \rangle \]

or

\[ \lambda^2 |\lambda \rangle = \lambda |\lambda \rangle \rightarrow (\lambda^2 - \lambda) |\lambda \rangle = 0 \]
\[ (\lambda^2 - \lambda) = 0 \rightarrow \lambda = 0, 1 \]

So projection operators are idempotent operators.
4.22.7 Operator Algebra

An operator for a two-state system is given by

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

where \(a\) is a number. Find the eigenvalues and the corresponding eigenkets.

In the \(\{|1\rangle, |2\rangle\}\) basis we have

$$H = \begin{pmatrix} a & a \\ a & -a \end{pmatrix}$$

The characteristic equation is

$$\det \begin{vmatrix} a - \lambda & a \\ a & -a - \lambda \end{vmatrix} = 0 = \lambda^2 - 2a^2$$

so that

$$\lambda_{\pm} = \pm \sqrt{2a}$$

To find the eigenkets we have

$$\hat{H} |+\rangle = \lambda_+ |+\rangle = \sqrt{2a} |+\rangle, \quad |+\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

which gives

$$\begin{pmatrix} a & a \\ a & -a \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \sqrt{2a} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$a \alpha + a \beta = \sqrt{2a} \alpha$$

$$a \alpha - a \beta = \sqrt{2a} \beta$$

so that

$$\beta = \left(\sqrt{2} - 1\right) a$$

Normalizing, we have

$$|+\rangle = \frac{1}{\sqrt{1.17}} \begin{pmatrix} 1 \\ 0.41 \end{pmatrix} = \frac{1}{\sqrt{1.17}} (|1\rangle + 0.41 |2\rangle)$$

and similarly (or using orthonormality),

$$|-\rangle = \frac{1}{\sqrt{6.81}} \begin{pmatrix} 1 \\ -2.41 \end{pmatrix} = \frac{1}{\sqrt{6.81}} (|1\rangle - 2.41 |2\rangle)$$

Since \(\langle + | -\rangle = 0\), they are orthogonal. We also have

$$|+\rangle \langle +| = \frac{1}{1.17} (|1\rangle \langle 1| + 0.17 |2\rangle \langle 2| + 0.41 |1\rangle \langle 2| + 0.41 |2\rangle \langle 1|)$$

$$|-\rangle \langle -| = \frac{1}{6.81} (|1\rangle \langle 1| + 5.81 |2\rangle \langle 2| - 2.41 |1\rangle \langle 2| - 2.41 |2\rangle \langle 1|)$$

so that

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

as it should.
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.

Suppose $\hat{Q} |q\rangle = q |q\rangle$. Then

$$\hat{Q}^2 |q\rangle = \hat{Q} \hat{Q} |q\rangle = \hat{Q} q |q\rangle = q^2 |q\rangle$$

Now assume that (induction proof)

$$\hat{Q}^n |q\rangle = q^n |q\rangle$$

This implies that

$$\hat{Q} \hat{Q}^{n-1} |q\rangle = \hat{Q} q^{n-1} |q\rangle = q^n |q\rangle$$

We then have

$$e^{\hat{Q}} |q\rangle = \left( \sum_{n=0}^{\infty} \frac{\hat{Q}^n}{n!} \right) |q\rangle = \left( \sum_{n=0}^{\infty} \frac{q^n}{n!} \right) = e^q |q\rangle$$

4.22.9 A Symmetric Matrix

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

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

Find the matrix $A$.

Since $A$ is a symmetric matrix there exists an orthogonal matrix $U$ such that

$$D = U A U^T$$

where $D$ is the diagonal matrix

$$D = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$$

The matrix $U^T$ is given by the normalized eigenvectors of $A$. i.e.,

$$U^T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 \end{pmatrix}$$
Thus,

\[ U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \end{pmatrix} \]

Since

\[ U^T = U^{-1} \]

we find that

\[ A = U^{-1} D (U^T)^{-1} = U^T D U \]

We thus obtain

\[ A = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 5 & -1 & 0 \\ 0 & -1 & 5 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \]

4.22.10 Determinants and Traces

Let \( A \) be an \( n \times n \) matrix. Show that

\[ \det(\exp(A)) = \exp(\text{tr}(A)) \]

Any \( n \times n \) matrix can be brought into triangular form by a similarity transformation. This means there is an invertible \( n \times n \) matrix \( R \) such that

\[ R^{-1} A R = T \]

where \( T \) is a triangular matrix with diagonal elements which are the eigenvalues of \( A \) (\( \lambda_i \)). Now we have

\[ A = RTR^{-1} \]

and therefore

\[ \exp A = \exp(RTR^{-1}) = \sum_n (RTR^{-1})^n = R \sum_n (T)^n R^{-1} = R \exp(T) R^{-1} \]

Since \( T \) is triangular, the diagonal elements of the \( k^{th} \) power of \( T \) are \( \lambda_i^k \) where \( k \) is a positive integer. Consequently, the diagonal elements of \( \exp(T) \) are \( \exp(\lambda_i) \).

Since the determinant of a triangular matrix is equal to the product of the diagonal elements, we find

\[ \det(\exp(T)) = \exp(\lambda_1 + \lambda_2 + \ldots + \lambda_n) = \exp(\text{tr}(T)) \]

Since

\[ \text{tr}(T) = \text{tr}(R^{-1} A R) = \text{tr}(A R R^{-1}) = \text{tr}(A) \]

and

\[ \det(\exp(T)) = \det(R \exp(T) R^{-1}) = \det(\exp(RTR^{-1})) = \det(\exp(A)) \]

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we get
\[ \det(\exp(A)) = \exp(\text{tr}(A)) \]

Another solution method:
\[ e^{(\text{tr}(A))} = e^{(\sum_n a_n)} = \prod e^{a_n} \]

where the \( a_n \) are the eigenvalues of \( A \). From 4.22.8 we have
if \( A|a_n\rangle = a_n|a_n\rangle \) then \( e^A|a_n\rangle = e^{a_n}|a_n\rangle \)

by Taylor expansion. Therefore
\[ \det e^A = \prod_n a'_n = \prod_n e^{a_n} = e^{\text{tr}A} \]

4.22.11 Function of a Matrix

Let
\[ A = \begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix} \]

Calculate \( \exp(\alpha A) \), \( \alpha \) real.

The matrix \( A \) is symmetric. Therefore, there exists an orthogonal matrix \( U \) such that \( UAU^{-1} \) is a diagonal matrix. The diagonal elements of \( UAU^{-1} \) are the eigenvalues of \( A \). Since \( A \) is symmetric, the eigenvalues are real. We set
\[ D = UAU^{-1} \]

with
\[ D = \begin{pmatrix} d_{11} & 0 \\ 0 & d_{22} \end{pmatrix} \]

Then
\[ \exp(D) = \begin{pmatrix} e^{d_{11}} & 0 \\ 0 & e^{d_{22}} \end{pmatrix} \]

It then follows that
\[ e^{\epsilon D} = \exp(\epsilon UAU^{-1}) = U \exp(\epsilon A)U^{-1} \]

Therefore
\[ \exp(\epsilon A) = U^{-1}e^{\epsilon D}U \]

The matrix \( U \) is constructed by means of the eigenvalues and normalized eigenvectors of \( A \). The eigenvalues of \( A \) are given by
\[ \lambda_1 = 1 \quad , \quad \lambda_2 = -3 \]

The corresponding eigenvectors are
\[ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad , \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \]
Consequently, matrix $U$ is given by

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

It follows that

$$U = U^{-1}$$

and

$$\exp(\varepsilon A) = U e^{\varepsilon D} U = \frac{1}{2} \begin{pmatrix} e^\varepsilon + e^{-3\varepsilon} & e^\varepsilon - e^{-3\varepsilon} \\ e^\varepsilon - e^{-3\varepsilon} & e^\varepsilon + e^{-3\varepsilon} \end{pmatrix}$$

### 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.

Since the matrix $A$ is symmetric the eigenvalues are real. The eigenvalues are determined by

$$\det(A - \lambda I) = 0$$

This gives the characteristic polynomial

$$-\lambda^3 + 12\lambda^2 - 21\lambda + 10 = 0$$

The eigenvalues are

$$\lambda_1 = 1 \quad , \quad \lambda_2 = 1 \quad , \quad \lambda_3 = 10$$

which correspond to the eigenvectors

$$u_1 = \begin{pmatrix} -1 \\ -2 \\ 0 \end{pmatrix}, \quad u_2 = \begin{pmatrix} -1 \\ 0 \\ -1 \end{pmatrix}, \quad u_3 = \begin{pmatrix} 2 \\ -1 \\ -2 \end{pmatrix}$$

We find

$$(u_1, u_3) = 0, \quad (u_2, u_3) = 0, \quad (u_1, u_2) = 1$$

so they are not orthogonal. To apply the Gram-Schmidt algorithm, we choose

$$u'_1 = u_1, \quad u'_2 = u_2 + \alpha u_1, \quad u'_3 = u_3$$

where

$$\alpha = -\frac{(u_1, u_2)}{(u_1, u_1)} = -\frac{1}{5}$$
Consequently,

\[ u'_2 = \begin{pmatrix} -4/5 \\ 2/5 \\ -1 \end{pmatrix} \]

The new set \( u_1, u'_2, u_3 \) are orthogonal.

### 4.22.13 Infinite Dimensions

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

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

Since

\[ \det(AB) = \det(A) \det(B), \quad \det(A) = \det(A^T), \quad \det(I) = 1 \]

we have

\[ \det(AA^T) = \det(A) \det(A^T) = \det(A^2) = \det(I) = 1 \]

Therefore the inverse of \( A \) exists and we have \( A^T = A^{-1} \) with \( A^{-1}A = AA^{-1} = I \).

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

The answer is no. We have a counterexample. Let

\[
A = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & \cdots \\
0 & 0 & 1 & 0 & 0 & \cdots \\
0 & 0 & 0 & 1 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
\end{pmatrix}
\]

Then the transpose matrix \( A^T \) of \( A \) is given by

\[
A^T = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & \cdots \\
1 & 0 & 0 & 0 & 0 & \cdots \\
0 & 1 & 0 & 0 & 0 & \cdots \\
0 & 0 & 1 & 0 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
\end{pmatrix}
\]

It follows that

\[
AA^T = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & \cdots \\
0 & 1 & 0 & 0 & 0 & \cdots \\
0 & 0 & 1 & 0 & 0 & \cdots \\
0 & 0 & 0 & 1 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
\end{pmatrix} = I
\]

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and

\[ A^T A = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & \ldots \\
0 & 1 & 0 & 0 & 0 & \ldots \\
0 & 0 & 1 & 0 & 0 & \ldots \\
0 & 0 & 0 & 1 & 0 \\
& & & & & \ldots
\end{pmatrix} \neq I \]

Consequently,

\[ AA^T \neq A^T A \]

### 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.

We have

\[ M = \begin{bmatrix}
0 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0
\end{bmatrix} \]

The eigenvalues are \( \lambda = 0, \pm \sqrt{2} \). The eigenvectors are

\[ |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad |+\sqrt{2}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}, \quad \left|-\sqrt{2}\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} \]

Therefore,

\[ \hat{P}_0 = |0\rangle \langle 0| = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}^+ = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \]

\[ \hat{P}_{\sqrt{2}} = |\sqrt{2}\rangle \langle \sqrt{2}| = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}^+ = \frac{1}{4} \begin{pmatrix} 1 & \sqrt{2} & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix} \]

\[ \hat{P}_{-\sqrt{2}} = |-\sqrt{2}\rangle \langle -\sqrt{2}| = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}^+ = \frac{1}{4} \begin{pmatrix} 1 & -\sqrt{2} & \sqrt{2} \\ -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \]

and then we have

\[ 0\hat{P}_0 + \sqrt{2}\hat{P}_{\sqrt{2}} - \sqrt{2}\hat{P}_{-\sqrt{2}} = \begin{bmatrix}
0 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0
\end{bmatrix} = M \]
4.22.15 Measurement Results

Given particles in state

\[ |\alpha\rangle = \frac{1}{\sqrt{83}} (-3|1\rangle + 5|2\rangle + 7|3\rangle) \]

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?

We have

\[ |\alpha\rangle = \frac{1}{\sqrt{83}} (-3|1\rangle + 5|2\rangle + 7|3\rangle) \]

where the \{|1\rangle, |2\rangle, |3\rangle\} basis is the set of vectors

\[ |1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \]

The observable

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

has eigenvectors \{|1\rangle, |2\rangle, |3\rangle\} and eigenvalues 2, 3, -6. The possible values of any measurement are the eigenvalues and the probabilities are given by

\[ P(2|\alpha\rangle) = \langle 1 | 1 \rangle^2 = \frac{1}{83} (-3 \langle 1 | 1 \rangle + 5 \langle 1 | 2 \rangle + 7 \langle 1 | 3 \rangle)^2 = \frac{9}{83} \]
\[ P(3|\alpha\rangle) = \langle 2 | 2 \rangle^2 = \frac{1}{83} (-3 \langle 2 | 1 \rangle + 5 \langle 2 | 2 \rangle + 7 \langle 2 | 3 \rangle)^2 = \frac{25}{83} \]
\[ P(-6|\alpha\rangle) = \langle 3 | 3 \rangle^2 = \frac{1}{83} (-3 \langle 3 | 1 \rangle + 5 \langle 3 | 2 \rangle + 7 \langle 3 | 3 \rangle)^2 = \frac{49}{83} \]

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.

We have

$$R^2 = \begin{bmatrix} 6 & -2 \\ -2 & 9 \end{bmatrix} \begin{bmatrix} 6 & -2 \\ -2 & 9 \end{bmatrix} = \begin{bmatrix} 40 & -30 \\ -30 & 85 \end{bmatrix}$$

so that

$$\langle R^2 \rangle = \langle \Psi | R^2 | \Psi \rangle = \begin{bmatrix} a \\ b \end{bmatrix}^\dagger \begin{bmatrix} 40 & -30 \\ -30 & 85 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = (a^* b^*) \begin{bmatrix} 40 & -30 \\ -30 & 85 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$$

$$= 40 |a|^2 + 85 |b|^2 - 60 \text{Re}(a^* b)$$

(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

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

The eigenvalues of $R$ are 5, 10. The corresponding eigenvectors are

$$|5\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix}, |10\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

Using these eigenvectors as a basis we have

$$|\Psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{\sqrt{5}} (2a + b) |5\rangle + \frac{1}{\sqrt{5}} (a - 2b) |10\rangle$$

We then have

$$\langle R^2 \rangle = \langle \Psi | R^2 | \Psi \rangle = (5)^2 P(5) + (10)^2 P(10) = (5)^2 |\langle 5 | \Psi \rangle|^2 + (10)^2 |\langle 10 | \Psi \rangle|^2$$

$$= \frac{25}{5} |2a + b|^2 + \frac{100}{5} |a - 2b|^2 = 40 |a|^2 + 85 |b|^2 - 60 \text{Re}(a^* b)$$

as before.

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

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

where $a$ and $b$ are both real numbers.

(a) Obviously, $\hat{A}$ has a degenerate spectrum. Does $\hat{B}$ also have a degenerate spectrum?
Since $\hat{A}$ is diagonal, its eigenvalues are $a, -a, -a$. For $\hat{B}$, the characteristic equation is

$$\left|\begin{array}{ccc}
  b - \lambda & 0 & 0 \\
  0 & -\lambda & -ib \\
  0 & ib & -\lambda \\
\end{array}\right| = 0 = \lambda^2 (b - \lambda) - b^2 (b - \lambda)$$

which gives eigenvalues $b, b, -b$. We note the two-fold degeneracy in each case.

(b) Show that $\hat{A}$ and $\hat{B}$ commute. Simple matrix multiplication gives

$$\hat{A}\hat{B} = \begin{pmatrix}
  ab & 0 & 0 \\
  0 & 0 & iab \\
  0 & -iab & 0 \\
\end{pmatrix} = \hat{B}\hat{A} \to [\hat{A}, \hat{B}] = 0$$

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

The fact that the operators commute says that they have a common set of eigenvectors. Let $|u^i\rangle$ be the eigenvector of $\hat{B}$ with eigenvalue $\lambda_i$, that is,

$$\hat{B}|u^i\rangle = \lambda_i|u^i\rangle$$

Therefore, we have

$$\begin{pmatrix}
  b & 0 & 0 \\
  0 & 0 & -ib \\
  0 & ib & 0 \\
\end{pmatrix} \begin{pmatrix}
  u_1^1 \\
  u_2^1 \\
  u_3^1 \\
\end{pmatrix} = \lambda_1 \begin{pmatrix}
  u_1^1 \\
  u_2^1 \\
  u_3^1 \\
\end{pmatrix} = b \begin{pmatrix}
  u_1^1 \\
  u_2^1 \\
  u_3^1 \\
\end{pmatrix}$$

which gives

$$bu_1^1 = bu_1^1, \quad -ibu_3^1 = bu_2^1, \quad ibu_2^1 = bu_3^1$$

We choose the solution

$$|u^1\rangle = |b\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |1\rangle$$

For $\lambda_2 = b$ (degenerate eigenvalue) we have the same equations as above and, in addition, must have $\langle u^1 | u^2 \rangle = 0$ (they must be orthogonal). If we choose $u_1^2 = 0$, then the other two equations imply $ibu_2^2 = bu_3^2$. If we choose $u_2^2 = 1$, then we get $u_3^2 = i$ so that

$$|u^2\rangle = |2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & i \end{pmatrix} = \frac{1}{\sqrt{2}} (|2\rangle + i |3\rangle)$$

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For the non-degenerate eigenvalue \(\lambda_3 = -b\), we must have \(\langle u^1 | u^3 \rangle = 0 = \langle u^2 | u^3 \rangle\) (orthogonal to the other two eigenvectors). If we choose \(u^1_3 = 0\) (guarantees \(\langle u^1 | u^3 \rangle = 0\)) and \(u^2_3 = 1\), then the equation \(ibu^3_2 = -bu^3_3\) says that \(u^3_3 = -i\), so that

\[
|u^3\rangle = |\beta\rangle = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 0 \\ 1 \\ -i \end{array} \right) = \frac{1}{\sqrt{2}} (|2\rangle - i|3\rangle)
\]

The set \{|1\rangle , |2\rangle , |3\rangle\} are also eigenvectors of \(\hat{A}\).

4.22.18 The World of Hard/Soft Particles

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

\[
\hat{O}_{\text{HARDNESS}} |h\rangle = |h\rangle , \quad \hat{O}_{\text{HARDNESS}} |s\rangle = -|s\rangle
\]

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

\[
\hat{O}_{\text{HARDNESS}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

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.

\[
\langle A | A \rangle = (\cos \varphi \langle h | h \rangle + e^{-i\varphi} \sin \theta \langle s | s \rangle) (\cos \theta |h\rangle + e^{i\varphi} \sin \theta |s\rangle)
\]

\[
= \cos^2 \varphi \langle h | h \rangle + e^{2i\varphi} \sin \varphi \cos \theta \langle h | s \rangle + e^{-2i\varphi} \sin \varphi \cos \theta \langle s | h \rangle + \sin^2 \theta \langle s | s \rangle
\]

\[
= \cos^2 \varphi + \sin^2 \theta = 1
\]

which says that the vector is normalized.

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

\[
|B\rangle = \alpha |h\rangle + \beta |s\rangle
\]

\[
\langle A | B \rangle = (\cos \varphi \langle h | h \rangle + e^{-i\varphi} \sin \theta \langle s | s \rangle) (\alpha \langle h \rangle + \beta \langle s \rangle) = 0
\]

\[
0 = \alpha \cos \theta + e^{-i\varphi} \beta \sin \theta \Rightarrow \beta = -e^{i\varphi} \alpha \cot \theta
\]

\[
\langle B | B \rangle = (\alpha^* \langle h | + \beta^* \langle s |) (\alpha \langle h \rangle + \beta \langle s \rangle) = |\alpha|^2 + |\beta|^2 = 1
\]

\[
|\alpha|^2 + \cot^2 \theta |\alpha|^2 = 1 \Rightarrow |\alpha|^2 = \frac{1}{1 + \cot^2 \theta} = \sin^2 \theta
\]

\[
\alpha = \sin \theta , \quad \beta = -e^{i\varphi} \cos \theta
\]

\[
|B\rangle = \sin \theta |h\rangle - e^{i\varphi} \cos \theta |s\rangle
\]
(c) Express $|h\rangle$ and $|s\rangle$ in the \{\{A\rangle, |B\rangle\} basis.

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

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

$$\langle h \mid A\rangle = \cos \theta = \langle A \mid h\rangle, \quad \langle h \mid B\rangle = \sin \theta = \langle B \mid h\rangle$$

$$\langle s \mid A\rangle = e^{i\varphi} \sin \theta = \langle A \mid s\rangle^*, \quad \langle s \mid B\rangle = -e^{i\varphi} \cos \theta = \langle B \mid s\rangle^*$$

$$|h\rangle = \langle A \mid h\rangle |A\rangle + \langle B \mid h\rangle |B\rangle = \cos \theta |A\rangle + \sin \theta |B\rangle$$

$$|s\rangle = \langle A \mid s\rangle |A\rangle + \langle B \mid s\rangle |B\rangle$$

$$e^{-i\varphi} \sin \theta |A\rangle - e^{-i\varphi} \cos \theta |B\rangle = e^{-i\varphi} (\sin \theta |A\rangle - \cos \theta |B\rangle)$$

$$|s\rangle = \sin \theta |A\rangle - \cos \theta |B\rangle$$

since overall phase factors are irrelevant.

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

$$P(h \mid A) = |\langle h \mid A\rangle|^2 = \cos^2 \theta$$

$$P(s \mid A) = |\langle s \mid A\rangle|^2 = \sin^2 \theta$$

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

$$\hat{H} = |h\rangle \langle h| - |s\rangle \langle s|$$

$$H = \begin{pmatrix} \langle A \mid \hat{H} \mid A\rangle & \langle A \mid \hat{H} \mid B\rangle \\ \langle B \mid \hat{H} \mid A\rangle & \langle B \mid \hat{H} \mid B\rangle \end{pmatrix}$$

$$= \begin{pmatrix} \langle A \mid h\rangle \langle h \mid A\rangle - \langle A \mid s\rangle \langle s \mid A\rangle & \langle A \mid h\rangle \langle h \mid B\rangle - \langle A \mid s\rangle \langle s \mid B\rangle \\ \langle B \mid h\rangle \langle h \mid A\rangle - \langle B \mid s\rangle \langle s \mid A\rangle & \langle B \mid h\rangle \langle h \mid B\rangle - \langle B \mid s\rangle \langle s \mid B\rangle \end{pmatrix}$$

$$= \begin{pmatrix} \cos^2 \theta - \sin^2 \theta & 2 \sin \theta \cos \theta \\ 2 \sin \theta \cos \theta & \sin^2 \theta - \cos^2 \theta \end{pmatrix}$$

or

$$\hat{H} = |h\rangle \langle h| - |s\rangle \langle s|$$

$$= (\cos \theta |A\rangle + \sin \theta |B\rangle) (\cos \theta \langle A\rangle + \sin \theta \langle B\rangle)$$

$$- (\sin \theta |A\rangle - \cos \theta |B\rangle) (\sin \theta \langle A\rangle - \cos \theta \langle B\rangle)$$

$$= \cos 2\theta |A\rangle \langle A| + \sin 2\theta |B\rangle \langle A| + \sin 2\theta |A\rangle \langle B| - \cos 2\theta |B\rangle \langle B|$$

In the \{\{A\rangle, |B\rangle\} basis

$$|A\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |B\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|A\rangle \langle A| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad |A\rangle \langle B| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$|B\rangle \langle A| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad |B\rangle \langle B| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

so that

$$\hat{H} = \cos 2\theta \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \sin 2\theta \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \sin 2\theta \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} - \cos 2\theta \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{pmatrix}$$
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. $|0\rangle \langle 1| + i|1\rangle \langle 0|$

   Not Hermitian: $(|0\rangle \langle 1| + i|1\rangle \langle 0|)^* = |1\rangle \langle 0| - i|0\rangle \langle 1| \neq |0\rangle \langle 1| + i|1\rangle \langle 0|$

2. $|0\rangle \langle 0| + |1\rangle \langle 1| + |2\rangle \langle 3| + |3\rangle \langle 2|$

   Hermitian: $(|0\rangle \langle 0| + |1\rangle \langle 1| + |2\rangle \langle 3| + |3\rangle \langle 2|)^* = |0\rangle \langle 0| + |1\rangle \langle 1| + |2\rangle \langle 3| + |3\rangle \langle 2|$

3. $(a|0\rangle + |1\rangle)^*(a|0\rangle + |1\rangle)$

   Hermitian: $(a|0\rangle + |1\rangle)^*(a|0\rangle + |1\rangle) = a^*a + 1 = |a|^2 + 1$ since real numbers are Hermitian.

4. $((a|0\rangle + b^*|1\rangle)^*(b|0\rangle - a^*|1\rangle))|2\rangle \langle 1| + |3\rangle \langle 3|$

   Hermitian: $((a|0\rangle + b^*|1\rangle)^*(b|0\rangle - a^*|1\rangle))|2\rangle \langle 1| + |3\rangle \langle 3|$

   $= |3\rangle \langle 3|$

5. $|0\rangle \langle 0| + i|1\rangle \langle 0| - i|0\rangle \langle 1| + |1\rangle \langle 1|$

   Hermitian: $(|0\rangle \langle 0| + i|1\rangle \langle 0| - i|0\rangle \langle 1| + |1\rangle \langle 1|)^* = |0\rangle \langle 0| - i|0\rangle \langle 1| + |1\rangle \langle 0| + i|1\rangle \langle 0| + |1\rangle \langle 1|$

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

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

The $\hat{K}$ matrix is

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

The eigenvalues follow from the characteristic equation

$$\det\begin{pmatrix}
1 - \lambda & 0 & 0 & 0 \\
0 & -\lambda & 2 & 0 \\
0 & 2 & -\lambda & 0 \\
0 & 0 & 0 & -1 - \lambda
\end{pmatrix} = 0 = (1 - \lambda)\left(-\lambda^2 (1 + \lambda) + 4 (1 + \lambda)\right)$$

$(1 - \lambda)(1 + \lambda)(2 + \lambda)(2 - \lambda) = 0 \Rightarrow \lambda_0 = 1, \lambda_1 = 2, \lambda_2 = -2, \lambda_3 = -1$

Thus, we can write

$$\hat{K} = 2|\lambda_1\rangle - 2|\lambda_2\rangle - 1|\lambda_3\rangle$$
where
\[
|\lambda_1\rangle = |0\rangle \\
|\lambda_1\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle) \\
|\lambda_2\rangle = \frac{1}{\sqrt{2}} (|1\rangle - |2\rangle) \\
|\lambda_3\rangle = |3\rangle
\]

(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?

Since
\[
\hat{B}^2 = \left( \frac{1}{\sqrt{2}} (\hat{I} + |\Psi\rangle \langle \Psi|) \right)^2 = \frac{1}{2} \left( \hat{I} + 3 |\Psi\rangle \langle \Psi| \right) \neq \hat{B}
\]
$\hat{B}$ is not a projection operator.

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

Clearly, $|\Psi\rangle$ is an eigenvector of $\hat{B}$ with eigenvalue $\sqrt{2}$, i.e.,
\[
\hat{B} |\Psi\rangle = \left( \frac{1}{\sqrt{2}} (\hat{I} + |\Psi\rangle \langle \Psi|) \right) |\Psi\rangle = \frac{1}{\sqrt{2}} (\hat{I} |\Psi\rangle + |\Psi\rangle \langle \Psi| |\Psi\rangle) \\
= \frac{\sqrt{2}}{\sqrt{2}} |\Psi\rangle = \sqrt{2} |\Psi\rangle
\]
Now we can write
\[
\hat{B} = \frac{1}{\sqrt{2}} (\hat{I} + |\Psi\rangle \langle \Psi|) = \sqrt{2} |\Psi\rangle \langle \Psi| + \frac{1}{\sqrt{2}} (\hat{I} - |\Psi\rangle \langle \Psi|)
\]
where it is understood that the term $\hat{I} - |\Psi\rangle \langle \Psi|$ can be further decomposed into the other three eigenvectors of $\hat{B}$ that are mutually orthogonal and orthogonal to $|\Psi\rangle$.

Label them as $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle$. Since these three eigenvectors are orthogonal to $|\Psi\rangle$ we then have
\[
\hat{B} |\varphi_j\rangle = \frac{1}{\sqrt{2}} (\hat{I} + |\Psi\rangle \langle \Psi|) |\varphi_j\rangle = \frac{1}{\sqrt{2}} |\varphi_j\rangle + \frac{1}{\sqrt{2}} |\Psi\rangle \langle \Psi| |\varphi_j\rangle = \frac{1}{\sqrt{2}} |\varphi_j\rangle
\]
i.e., the other three eigenvalues are $1/\sqrt{2}$. The three states are degenerate. Since $\hat{B}$ does not provide any restraining conditions other than orthogonality with $|\Psi\rangle$, we cannot specify the other eigenvectors any further.
4.22.20 A 2-Dimensional Hilbert Space

Consider a 2-dimensional Hilbert space spanned by an orthonormal basis \{\langle \uparrow \rangle, \langle \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

\[ \hat{S}_x = \frac{\hbar}{2} (\langle \uparrow \rangle \langle \downarrow \rangle + \langle \downarrow \rangle \langle \uparrow \rangle), \quad \hat{S}_y = \frac{\hbar}{2i} (\langle \uparrow \rangle \langle \downarrow \rangle - \langle \downarrow \rangle \langle \uparrow \rangle), \quad \hat{S}_z = \frac{\hbar}{2} (\langle \uparrow \rangle \langle \uparrow \rangle - \langle \downarrow \rangle \langle \downarrow \rangle) \]

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

\[ \hat{S}_x = \frac{\hbar}{2} (\langle \uparrow \rangle \langle \downarrow \rangle + \langle \downarrow \rangle \langle \uparrow \rangle), \quad \hat{S}_y = \frac{\hbar}{2i} (\langle \uparrow \rangle \langle \downarrow \rangle - \langle \downarrow \rangle \langle \uparrow \rangle), \quad \hat{S}_z = \frac{\hbar}{2} (\langle \uparrow \rangle \langle \uparrow \rangle - \langle \downarrow \rangle \langle \downarrow \rangle) \]

and similarly for \(\hat{S}_y\) and \(\hat{S}_z\).

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

\[ \begin{bmatrix} \hat{S}_x \end{bmatrix} = \begin{bmatrix} \langle \uparrow | \hat{S}_x | \uparrow \rangle & \langle \uparrow | \hat{S}_x | \downarrow \rangle \\ \langle \downarrow | \hat{S}_x | \uparrow \rangle & \langle \downarrow | \hat{S}_x | \downarrow \rangle \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \]

\[ \hat{S}_y = \frac{\hbar}{2i} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \quad \hat{S}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \]

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

\[ \begin{bmatrix} \hat{S}_x, \hat{S}_y \end{bmatrix} = \frac{\hbar^2}{4i} \begin{bmatrix} \langle \uparrow | \hat{S}_x | \uparrow \rangle \langle \downarrow \rangle + \langle \downarrow | \hat{S}_x | \downarrow \rangle \langle \uparrow \rangle & \langle \uparrow | \hat{S}_x | \downarrow \rangle \langle \downarrow \rangle - \langle \downarrow | \hat{S}_x | \uparrow \rangle \langle \uparrow \rangle \\ \langle \downarrow | \hat{S}_x | \uparrow \rangle \langle \downarrow \rangle + \langle \downarrow | \hat{S}_x | \downarrow \rangle \langle \uparrow \rangle & \langle \downarrow | \hat{S}_x | \downarrow \rangle \langle \downarrow \rangle - \langle \uparrow | \hat{S}_x | \uparrow \rangle \langle \uparrow \rangle \end{bmatrix} = \frac{\hbar^2}{4i} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \]

\[ \begin{bmatrix} \hat{S}_x, \hat{S}_z \end{bmatrix} = \frac{\hbar^2}{4i} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{i\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = i\hbar \hat{S}_z \]

Now let

\[ |\pm\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle \pm |\downarrow\rangle) \]

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

Note that these vectors are eigenvectors of \(\hat{S}_x\). Clearly, we have

\[ \langle + | + \rangle = \frac{1}{2} (\langle \uparrow | + \downarrow \rangle \langle \uparrow | + \downarrow \rangle) = \frac{1}{2}(1 + 1) = 1 = \langle - | - \rangle \]
\[ \langle + | - \rangle = \frac{1}{2} (\langle \uparrow | + \downarrow \rangle \langle \uparrow | - \downarrow \rangle) = \frac{1}{2}(1 - 1) = 0 = \langle - | + \rangle \]

so they form an orthonormal basis.
(e) Find the matrix representations of these operators in the \( \{|+\rangle, |-\rangle\} \) basis.

\[
\begin{align*}
\hat{S}_x \pm &= \frac{\hbar}{2} \left( \begin{array}{cc}
(\langle \uparrow \rangle + \langle \downarrow \rangle) (\langle \uparrow \rangle (\uparrow) + \langle \downarrow \rangle (\downarrow)) & (\langle \uparrow \rangle + \langle \downarrow \rangle) (\langle \uparrow \rangle (\downarrow) + \langle \downarrow \rangle (\uparrow)) \\
(\langle \uparrow \rangle - \langle \downarrow \rangle) (\langle \uparrow \rangle (\uparrow) - \langle \downarrow \rangle (\downarrow)) & (\langle \uparrow \rangle - \langle \downarrow \rangle) (\langle \uparrow \rangle (\downarrow) - \langle \downarrow \rangle (\uparrow))
\end{array} \right) \\
&\hspace{1cm} = \frac{\hbar}{4} \left( \begin{array}{cc}
1 + 1 & -1 + 1 \\
1 - 1 & -1 - 1
\end{array} \right) = \frac{\hbar}{2} \left( \begin{array}{cc}
1 & 0 \\
0 & -1
\end{array} \right) = \hat{S}_x
\end{align*}
\]

Clearly, \( \hat{S}_x \) is diagonal in its own basis.

\[
\begin{align*}
\hat{S}_y \pm &= \frac{\hbar}{2} \left( \begin{array}{cc}
(\langle \uparrow \rangle + \langle \downarrow \rangle) (\langle \uparrow \rangle (\downarrow) + \langle \downarrow \rangle (\uparrow)) & (\langle \uparrow \rangle + \langle \downarrow \rangle) (\langle \uparrow \rangle (\uparrow) + \langle \downarrow \rangle (\downarrow)) \\
(\langle \uparrow \rangle - \langle \downarrow \rangle) (\langle \uparrow \rangle (\downarrow) - \langle \downarrow \rangle (\uparrow)) & (\langle \uparrow \rangle - \langle \downarrow \rangle) (\langle \uparrow \rangle (\uparrow) - \langle \downarrow \rangle (\downarrow))
\end{array} \right) \\
&\hspace{1cm} = \frac{\hbar}{4} \left( \begin{array}{cc}
1 - 1 & -1 + 1 \\
1 + 1 & -1 - 1
\end{array} \right) = \frac{\hbar}{2} \left( \begin{array}{cc}
0 & -1 \\
1 & 0
\end{array} \right) = -\hat{S}_y
\end{align*}
\]

\[
\begin{align*}
\hat{S}_z \pm &= \frac{\hbar}{2} \left( \begin{array}{cc}
(\langle \uparrow \rangle + \langle \downarrow \rangle) (\langle \uparrow \rangle (\uparrow) - \langle \downarrow \rangle (\downarrow)) & (\langle \uparrow \rangle + \langle \downarrow \rangle) (\langle \uparrow \rangle (\downarrow) - \langle \downarrow \rangle (\uparrow)) \\
(\langle \uparrow \rangle - \langle \downarrow \rangle) (\langle \uparrow \rangle (\uparrow) - \langle \downarrow \rangle (\downarrow)) & (\langle \uparrow \rangle - \langle \downarrow \rangle) (\langle \uparrow \rangle (\downarrow) - \langle \downarrow \rangle (\uparrow))
\end{array} \right) \\
&\hspace{1cm} = \frac{\hbar}{4} \left( \begin{array}{cc}
1 - 1 & 1 + 1 \\
1 + 1 & 1 - 1
\end{array} \right) = \frac{\hbar}{2} \left( \begin{array}{cc}
0 & 1 \\
1 & 0
\end{array} \right) = \hat{S}_z
\end{align*}
\]

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

\[
\hat{S}_{x(\dagger)} = U^\dagger \hat{S}_{x(\pm)} U , \quad \hat{S}_{y(\dagger)} = U^\dagger \hat{S}_{y(\pm)} U , \quad \hat{S}_{z(\dagger)} = U^\dagger \hat{S}_{z(\pm)} U
\]

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

The unitary matrix which diagonalizes \( \hat{S}_x \) is given by the eigenvectors of \( \hat{S}_x \), i.e.,

\[
U = \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right)
\]

Therefore, we want

\[
U^\dagger = U = \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) = U^{-1}
\]

and

\[
\begin{align*}
U^\dagger \left[ \hat{S}_x \right] \pm U &= \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) \frac{\hbar}{2} \left( \begin{array}{cc}
0 & 1 \\
1 & 0
\end{array} \right) \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) \\
&= \frac{\hbar}{4} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) \left( \begin{array}{cc}
0 & 1 \\
1 & 0
\end{array} \right) \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) = \hat{S}_z
\end{align*}
\]

\[
\begin{align*}
U^\dagger \left[ \hat{S}_y \right] \pm U &= \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) \frac{\hbar}{2} \left( \begin{array}{cc}
0 & 1 \\
1 & 0
\end{array} \right) \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) \\
&= \frac{\hbar}{4} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) \left( \begin{array}{cc}
0 & 1 \\
1 & 0
\end{array} \right) \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right) = \hat{S}_y
\end{align*}
\]

\[48\]
as expected.

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 \( \hat{S}_\dag \hat{S}_+ = \hat{S}_- \).

\[
\hat{S}_\pm = \frac{1}{2} \left( \hat{S}_x \pm i \hat{S}_y \right) = \frac{1}{2} \left( \frac{\hbar}{i} \langle 0 | - | 1 \rangle \langle 1 | + | 0 \rangle | \uparrow \rangle \right) + \frac{\hbar}{2} \left( \langle -1 | -1 | \downarrow \rangle \langle 1 | + 1 | \uparrow \rangle \right) \\
\hat{S}_+ = \frac{1}{2} | \uparrow \rangle \langle \downarrow | \ , \ \hat{S}_- = \frac{1}{2} | \downarrow \rangle \langle \uparrow | \\
\]

(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
\[
\langle \uparrow | \hat{S}_+ , \langle \downarrow | \hat{S}_+ , \langle \uparrow | \hat{S}_- , \langle \downarrow | \hat{S}_- \\
\hat{S}_+ | \uparrow \rangle = \left( \frac{\hbar}{2} | \uparrow \rangle \langle \downarrow | \downarrow \rangle = \frac{\hbar}{2} | \uparrow \rangle \right) \ , \ \hat{S}_- | \uparrow \rangle = \left( \frac{\hbar}{2} | \downarrow \rangle \langle \uparrow | \uparrow \rangle = \frac{\hbar}{2} | \downarrow \rangle \right)  \\
\hat{S}_+ | \downarrow \rangle = \left( \frac{\hbar}{2} | \uparrow \rangle \langle \downarrow | \downarrow \rangle = 0 \right) \ , \ \hat{S}_- | \downarrow \rangle = \left( \frac{\hbar}{2} | \downarrow \rangle \langle \uparrow | \downarrow \rangle = 0 \right) \\
\left( \hat{S}_+ | \uparrow \rangle \right)^\dagger = \langle \downarrow | \hat{S}_- = 0 \ , \ \left( \hat{S}_+ | \downarrow \rangle \right)^\dagger = \langle \uparrow | \hat{S}_- = \frac{\hbar}{2} | \downarrow \rangle \\
\left( \hat{S}_- | \uparrow \rangle \right)^\dagger = \langle \downarrow | \hat{S}_+ = \frac{\hbar}{2} | \uparrow \rangle \ , \ \left( \hat{S}_- | \downarrow \rangle \right)^\dagger = \langle \uparrow | \hat{S}_+ = 0 \\
\]

### 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 \( M^2 = M_x^2 + M_y^2 + M_z^2 \).

The matrices \( M_i \) represent the \( i^{th} \) component of some angular momentum operator \( \vec{J} \) in some basis \( \{\alpha, j, m\} \). For each set of values \( (\alpha, j) \), there are \( 2j + 1 \) different values of \( m \). There can be basis vectors with the same value of \( j \) but different values of \( m \).

Since there is one eigenvector with \( m = 2 \), there must be just one set of vectors \( \{\alpha, 2, m\} \). There are therefore 5 eigenvectors with the eigenvalue \( 2(2 + 1)\hbar^2 = \)
6\hbar^2 of \textit{J}^2(M^2). This set of vectors produces the eigenvalue \( m = 1 \) just once. But it occurs 28 times. There must therefore exist 27 sets of vectors \( \{\alpha, 1, m\} \). There are therefore \( 27 \times 3 = 81 \) eigenvectors with the eigenvalue \( 1(1+1)\hbar^2 = 2\hbar^2 \) of \( \textit{J}^2 \).

We now have \( 27 + 1 = 28 \) vectors that produce the eigenvalue \( m = 0 \). However, it occurs 70 times. There must therefore be \( 70 - 28 = 42 \) vectors \( \{\alpha, 0, 0\} \) with eigenvalue \( 0 \) of \( \textit{J}^2 \).

The eigenvalue \( 3\hbar/2 \) occurs 8 times. There are therefore 8 sets of vectors \( \{\alpha, 3/2, m\} \) and the eigenvalue \( 3/2(3/2 + 1)\hbar^2 = 15\hbar^2/4 \) occurs \( 4 \times 8 = 32 \) times. This set of vectors produces \( m = 1/2 \) 8 times. Since it occurs 56 times, there must be \( 56 - 8 = 48 \) vectors \( \{\alpha, 1/2, m\} \). They produce the eigenvalue \( 1/2(1/2 + 1)\hbar^2 = 3\hbar^2/4 \) \( 48 \times 2 = 96 \) times.

**Summary:**

<table>
<thead>
<tr>
<th>Value</th>
<th>6\hbar^2</th>
<th>15\hbar^2/4</th>
<th>2\hbar^2</th>
<th>3\hbar^2/4</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Times</td>
<td>5</td>
<td>32</td>
<td>81</td>
<td>96</td>
<td>42</td>
</tr>
</tbody>
</table>

for a total of 256.

### 4.22.22 Operator Properties

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

Equation (4.117) in the text gives this definition.

If we have an operator \( \hat{Q} \) where the adjoint satisfies the relation

\[
\langle q | \hat{Q}^\dagger | p \rangle^* = \langle p | \hat{Q} | q \rangle = (\langle p | \hat{Q} | q \rangle)^*
\]

then \( \hat{Q} \) is a Hermitian or self-adjoint operator.

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

In quantum mechanics, a Hermitian operator has \( \hat{Q}^\dagger = \hat{Q} \).

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

We have

\[
\int_{-\infty}^{\infty} \phi^*(x) \frac{d\psi(x)}{dx} \, dx = [\phi^*(x)\psi(x)]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\phi^*(x)}{dx} \psi(x) \, dx
\]

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Now the boundary term vanishes because both $\phi(x)$ and $\psi(x)$ vanish at $x = \pm \infty$. We then have
\[
\int_{-\infty}^{\infty} \phi^*(x) \frac{d\psi(x)}{dx} \, dx = -\int_{-\infty}^{\infty} \left( \frac{d\phi(x)}{dx} \right)^* \psi(x) \, dx
\]
which says that
\[
\left( \frac{d}{dx} \right)^\dagger = -\frac{d}{dx}
\]
(d) Prove that for any two operators $A$ and $B$, $(AB)^\dagger = B^\dagger A^\dagger$

This is a bit tedious using integrals (try it with Dirac language). You need to keep using the definition of the conjugate.
\[
\left( \int \psi_1^*(AB)\psi_2 \, dx \right)^* = \int \psi_2^*(AB)^\dagger \psi_1 \, dx
\]
Now, recognize that $B\psi_2$ is just some other function, which we can call $\psi_3$. Using the definition,
\[
\left( \int \psi_1^* A\psi_3 \, dx \right)^* = \int \psi_3^* A^\dagger \psi_1 \, dx
\]
Now do the same thing again, with $A^\dagger \psi_1 = \psi_4$, and write
\[
\int \psi_3^* \psi_4 \, dx = \left( \int \psi_4^* \psi_3 \, dx \right)^*
\]
(because $\psi_3^*$ and $\psi_4^*$ commute, and taking a * outside the whole integral). Re-using $\psi_3 = B\psi_2$ brings in $B^\dagger$, and reordering terms brings $B^\dagger A^\dagger$ together in the middle. Thus we show that $(AB)^\dagger = B^\dagger A^\dagger$

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.
We have
\[
\frac{\partial}{\partial t} \langle O \rangle = \frac{\partial}{\partial t} \langle \psi | O | \psi \rangle \\
= \left[ \frac{\partial}{\partial t} \langle \psi | \right] O | \psi \rangle + \langle \psi | O \left[ \frac{\partial}{\partial t} | \psi \rangle \right] \\
= -\langle \psi | \frac{1}{i\hbar} H | \psi \rangle O | \psi \rangle + \langle \psi | O \left[ \frac{1}{i\hbar} H | \psi \rangle \right] \\
= \frac{i}{\hbar} \langle \psi | (HO - OH) | \psi \rangle
\]
which says that
\[
\frac{\partial}{\partial t} \langle O \rangle = \frac{i}{\hbar} \langle [H, O] \rangle
\]

Use this result to derive Ehrenfest's relations, which show that classical mechanics still applies to expectation values:
\[
m \frac{\partial}{\partial t} \langle \vec{x} \rangle = \langle \vec{p} \rangle, \quad \frac{\partial}{\partial t} \langle \vec{p} \rangle = -\langle \nabla V \rangle
\]

We have
\[
\frac{d}{dt} \langle x \rangle = \frac{i}{\hbar} \langle [H, x] \rangle = \frac{i}{\hbar} \langle \frac{1}{2m} [p_x^2, x] \rangle \\
= \frac{i}{2m\hbar} \langle (p_x^2, x) - xp_x^2 \rangle = \frac{i}{2m\hbar} \langle (p_x^2, x) - p_x^2x + p_x x p_x - x p_x x \rangle \\
= \frac{i}{2m\hbar} \langle [p_x, x] + [p_x, x] p_x \rangle = \frac{i}{2m\hbar} \langle [-2ip_x x] \rangle \\
= \langle \frac{p_x}{m} \rangle
\]
Similarly for \( y \) and \( z \) components. Therefore we have
\[
m \frac{\partial}{\partial t} \langle \vec{x} \rangle = \langle \vec{p} \rangle
\]

Now we have
\[
\frac{d}{dt} \langle p_x \rangle = \frac{i}{\hbar} \langle [H, p_x] \rangle = \frac{i}{\hbar} \langle [V(x), p_x] \rangle \\
= \frac{i}{\hbar} \langle \hbar \frac{\partial V(x)}{\partial x} \rangle = -\langle \frac{\partial V(x)}{\partial x} \rangle
\]
Similarly for \( y \) and \( z \) components. Therefore we have
\[
\frac{\partial}{\partial t} \langle \vec{p} \rangle = -\langle \nabla V \rangle
\]
4.22.24 Solution of Coupled Linear ODEs

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

First we compute the eigenvalues of \( A \):

\[
\det(A - \lambda I) = \det \begin{pmatrix}
-\lambda & 1 & 1 \\
1 & -\lambda & 1 \\
1 & 1 & -\lambda
\end{pmatrix} = -\lambda^3 + 3\lambda + 2 = 0
\]

Since \( A \) is symmetric we know that all of its eigenvalues are real. By inspections, we can see that \( \lambda = -1 \) and \( \lambda = 2 \) are eigenvalues and so we can solve for the third:

\[-(\lambda + 1)(\lambda - 2)(\lambda - x) = -\lambda^3 + \lambda^2 + 2\lambda + x\lambda^2 - x\lambda - 2x = -\lambda^3 + 3\lambda + 2 \]

Hence, we find that \( x = -1 \) so that eigenvalue is repeated. Solving for the eigenvectors using

\[
Ax = \begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2 \\
x_3
\end{pmatrix} = \begin{pmatrix}
x_2 + x_3 \\
x_1 + x_3 \\
x_1 + x_2
\end{pmatrix} = \lambda \begin{pmatrix}
x_1 \\
x_2 \\
x_3
\end{pmatrix}
\]

we find for \( \lambda = -1 \),

\[
\begin{pmatrix}
x_2 + x_3 \\
x_1 + x_3 \\
x_1 + x_2
\end{pmatrix} = \lambda \begin{pmatrix}
-x_1 \\
-x_2 \\
-x_3
\end{pmatrix}
\]

which is satisfied as long as \( x_1 = -x_2 - x_3 \). Hence we have two linearly independent solutions

\[
v_{-1,1} = \frac{1}{2} \begin{pmatrix}
-2 \\
1 \\
1
\end{pmatrix}, \quad v_{-1,2} = \frac{1}{\sqrt{2}} \begin{pmatrix}
0 \\
1 \\
-1
\end{pmatrix}
\]

where with a little foresight we have chosen an orthogonal pair of eigenvectors. Likewise for \( \lambda = 2 \),

\[
\begin{pmatrix}
x_2 + x_3 \\
x_1 + x_3 \\
x_1 + x_2
\end{pmatrix} = 2 \lambda \begin{pmatrix}
x_1 \\
x_2 \\
x_3
\end{pmatrix}
\]

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or
\[
x_1 = \frac{1}{2}(x_2 + x_3)
\]
\[
\frac{1}{2}(x_2 + 3x_3) = 2x_2
\]
\[
3x_3 = 3x_2
\]
which gives
\[
v_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}
\]
Hence the unitary matrix which diagonalizes \( A \) is given by the eigenvectors as
\[
P = \begin{pmatrix}
\frac{-2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}}
\end{pmatrix}
\]
Since \( A \) is symmetric we also have \( P^{-1} = P^T \). Therefore
\[
A = \begin{pmatrix}
\frac{-2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}}
\end{pmatrix}
\begin{pmatrix}
-1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 2
\end{pmatrix}
\begin{pmatrix}
\frac{-2}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}}
\end{pmatrix}
\]
Now the formal solution to the differential equation is
\[
x(t) = e^{A(t)}x(0)
\]
We then have
\[
e^{A(t)} = \begin{pmatrix}
\frac{-2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}}
\end{pmatrix}
\begin{pmatrix}
e^{-t} & 0 & 0 \\
0 & e^{-t} & 0 \\
0 & 0 & e^{2t}
\end{pmatrix}
\begin{pmatrix}
\frac{-2}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}}
\end{pmatrix}
\]
\[
= \begin{pmatrix}
\frac{2}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} \\
-\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & \frac{2}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} \\
-\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & \frac{2}{3}e^{-t} + \frac{1}{3}e^{2t}
\end{pmatrix}
\]
and finally
\[
x(t) = \begin{pmatrix}
\frac{2}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} \\
-\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & \frac{2}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} \\
-\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & \frac{2}{3}e^{-t} + \frac{1}{3}e^{2t}
\end{pmatrix}x(0)
\]
(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 \((\lambda_i, v_i)\) are the eigenvalue-eigenvector pairs for \(A\) and the \(c_i\) are coefficients written in terms of the \(x(0)\).

Suppose that

\[
x(0) = \begin{pmatrix} a \\ b \\ c \end{pmatrix}
\]

Then using

\[
P^{-1} = \begin{pmatrix} -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix}
\]

we have

\[
\begin{pmatrix} c_{-1,1} \\ c_{-1,2} \\ c_2 \end{pmatrix} = \begin{pmatrix} -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}
\]

so

\[
x(t) = e^{-t} \left( -\frac{2}{\sqrt{6}}a + \frac{1}{\sqrt{6}}b + \frac{1}{\sqrt{6}}c \right) v_{-1,1} + e^{-t} \left( \frac{1}{\sqrt{2}}b - \frac{1}{\sqrt{2}}c \right) v_{-1,2} + e^{2t} \left( \frac{1}{\sqrt{3}}a + \frac{1}{\sqrt{3}}b + \frac{1}{\sqrt{3}}c \right) v_2
\]

### 4.22.25 Spectral Decomposition Practice

Find the spectral decomposition of the matrix

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

First we find the eigenvalues:

\[
\det (A - \lambda I) = \det \begin{pmatrix} 1 - \lambda & 0 & 0 \\ 0 & -\lambda & i \\ 0 & -i & -\lambda \end{pmatrix} = (1 - \lambda)\lambda^2 - 1 - \lambda = 0
\]

so we are looking for the roots of the equation

\[
(1 - \lambda)\lambda^2 - 1 - \lambda = (1 - \lambda)(1 - \lambda^2) = 0
\]

We have \(\lambda = 1\) (twice) and \(\lambda = -1\). For \(\lambda = 1\) we have to solve

\[
\begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & i \\ 0 & -i & -1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0
\]

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This clearly has the solution
\[
\begin{pmatrix}
1 \\
0 \\
0
\end{pmatrix}
\]
and also
\[-b + ic = 0 \ , \ -ib - c = 0 \rightarrow b = ic\]
Hence, if we choose \(a = 0\) in this case we have for \(\lambda = 1\)
\[
\begin{pmatrix}
1 \\
0 \\
0
\end{pmatrix}, \ \frac{1}{\sqrt{2}} \begin{pmatrix}
0 \\
i \\
1
\end{pmatrix}
\]
as the two orthonormal eigenvectors. The for \(\lambda = -1\), we have
\[
\begin{pmatrix}
2 & 0 & 0 \\
0 & 1 & i \\
0 & -i & 1
\end{pmatrix} \begin{pmatrix}
a \\
b \\
c
\end{pmatrix} = 0
\]
for which we will choose \(a = 0\) again and solve
\[-b + ic = 0 \ , \ -ib + c = 0 \rightarrow b = -ic\]
Then for \(\lambda = -1\) we have
\[
\frac{1}{\sqrt{2}} \begin{pmatrix}
0 \\
-i \\
1
\end{pmatrix}
\]
We then have the projection operators
\[
P_{-1} = \frac{1}{2} \begin{pmatrix}
-1 & 0 & 0 \\
0 & i & 1 \\
0 & -i & 1
\end{pmatrix} = \frac{1}{2} \begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & -i \\
0 & i & 1
\end{pmatrix}
\]
\[
P_{1} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix} + \frac{1}{2} \begin{pmatrix}
i \\
0 & -i & 1 \\
1 & 0 & 1
\end{pmatrix} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1/2 & i/2 \\
0 & -i/2 & 1/2
\end{pmatrix} + \begin{pmatrix}
0 & 0 & 0 \\
0 & 1/2 & -i/2 \\
0 & i/2 & 1/2
\end{pmatrix}
\]
and the spectral decomposition
\[
A = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1/2 & i/2 \\
0 & -i/2 & 1/2
\end{pmatrix} - \begin{pmatrix}
0 & 0 & 0 \\
0 & 1/2 & -i/2 \\
0 & i/2 & 1/2
\end{pmatrix}
\]
which is easily seen to be valid. Just for fun, we can also verify
\[
P_{1}P_{-1} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1/2 & i/2 \\
0 & -i/2 & 1/2
\end{pmatrix} \begin{pmatrix}
0 & 0 & 0 \\
0 & 1/2 & -i/2 \\
0 & i/2 & 1/2
\end{pmatrix} = 0
\]
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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 $I - P$.

We simply have

$$(1 - P)(1 - P) = 1 - 2P + P^2 = 1 - P$$

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

Since $P$ is Hermitian, we can decompose any state vector $|\Psi_a\rangle$ as

$$|\Psi_a\rangle = c_0 |0\rangle + c_1 |1\rangle$$

where

$$P |0\rangle = 0 \quad , \quad P |1\rangle = |1\rangle$$

Then

$$\langle \Psi_a | P |\Psi_a\rangle = |c_1|^2$$

and if $|\Psi_a\rangle$ is normalized, then $0 \leq |c_1|^2 \leq 1$.

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 $\sigma_i$ 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).

We have

$$P^+ P = P^2 = P$$

so the singular values of $P$ are either 0 or 1. Since $u_i^+ A^+ A u_i = \sigma_i^2$ is the square of the norm of the vector obtained by letting $A$ act on $u_i$, it follows that the action of an orthogonal projection operator never lengthens a vector.

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

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

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

First we find its eigenvalues, which are the roots of the equation

$$-\lambda(1-\lambda) = 0 \rightarrow \lambda = 0, 1$$

The corresponding eigenvectors are

$$\lambda = 0 \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \lambda = 1 \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We note that these are not orthogonal, and indeed, if we compute

$$P_0 = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad P_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

we find

$$\sum_i \lambda_i P_i = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \neq N$$

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

We compute

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

The eigenvalues of this matrix satisfy

$$(1-\lambda)^2 = 1 \rightarrow 1-\lambda = \pm 1$$

so the eigenvalues are 0 and 2. The singular values of $N$ are thus 0 and $\sqrt{2}$, meaning that there exists a unit vector the gets lengthened by the action of $N$. Indeed if we consider the normalized eigenvector of $N^T N$ with eigenvalue 2.

$$u_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

we find

$$Nu_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 2 \end{pmatrix}$$

The norm of this vector is now

$$\sqrt{u_2^T N u_2} = \sqrt{2}$$

The action of $N$ clearly projects onto the linear span of $(01)^T$. However, it does not project orthogonally along the $(01)^T$ direction, as can be seen.
from the fact that vectors parallel to that direction are in the nullspace of $N$. It follows that some vectors will have long shadows when projected in this oblique fashion.

The extreme example is the vector $u_2$ written above, which is in fact perpendicular to the direction of projection. Hence $u_2$, the unit vector along $(11)^T$, and $Nu_2$ can be arranged as a right isosceles triangle.
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 \( P(A) \).

The total number of possibilities is \( N = 6 \times 6 = 36 \), which is the number of pairs of the form \((i, j)\) with \(1 \leq i, j \leq 6\). The pairs with \(i < j\) are given by \( N_A = 15\), namely,

\[
(5, 6), (4, 5), (4, 6), (3, 4), (3, 5), (3, 6), (1, 5), (1, 6)
\]

Thus,

\[
P(A) = \frac{N_A}{N} = \frac{15}{36} = 0.417
\]

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

There are \(6^3 = 216\) possible outcomes of this experiment, as each die has 6 possible faces. You get a sum of 9 with outcomes such as \((1, 2, 6), (2, 1, 6), (3, 3, 3)\) and so on. Tedious enumeration reveals that there are 25 such triples, so

\[
P(9) = \frac{25}{216} = 0.1157
\]
A similar tedious enumeration show that there are 27 triples, such as 
\((1,3,6),(2,4,4)\) and so on, that sum to 10. So 
\[
P(10) = \frac{27}{216} = 0.125 > P(9)
\]

(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

Let \(A\) denote the first event and \(B\) the second event. Then \(\sim A\) is the event that no 6 is shown. There are \(6^4\) equally likely outcomes, and \(5^4\) of these show no 6. Hence
\[
P(A) = 1 - P(\sim A) = 1 - \left(\frac{5}{6}\right)^4 = \frac{671}{1296} = 0.518
\]

Likewise, \(\sim B\) is the event that no double 6 is shown. There are \(36^4\) equally likely outcomes, and \(35^4\) of these show no double 6. Hence
\[
P(B) = 1 - P(\sim B) = 1 - \left(\frac{35}{36}\right)^4 = 0.491
\]

Since \(P(A) > P(B)\), the first event is more likely.

(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) \(P(\text{dry})\)
(2) \(P(\text{dry AND windy})\)
(3) \(P(\text{wet OR windy})\)

\[
(1) P(\text{dry}) = P(\sim \text{wet}) = 1 - P(\text{wet}) = 1 - 0.3 = 0.7
\]
\[
(2) P(\text{dry AND windy}) = P(\text{windy}) - P(\sim \text{dry AND windy}) = P(\text{windy}) - P(\text{wet AND windy}) = 0.91 - 0.2 = 0.71
\]
\[
(3) P(\text{wet OR windy}) = P(\text{wet}) + P(\text{windy}) - P(\text{wet AND windy}) = 0.4 + 0.91 - 0.71 = 0.6
\]

(c) 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?

We have
\[
P(H \lor S) = P(H) + P(S) - P(H \land S) = 0.91 + 0.95 - 0.88 = 0.98
\]

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(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?

There are 36 outcomes and in 15 the right-hand score is larger. So

\[ P(\text{RH larger}) = \frac{15}{36} \]

Now suppose you roll the left-hand die first and it shows 5. Clearly it is not 15/36. In fact only 1 outcome will do - it must show a 6. So the required probability is 1/6. This is a special case of the general observation that if conditions change then results change.

More rigorous solution: We have the rule

\[ P(A \land B) = P(A|B)P(B) \]

Thus,

\[ P(R \text{ larger}|L \text{ shows 5}) = \frac{P(R \text{ shows 6 and L shows 5})}{P(L \text{ shows 5})} = \frac{1/36}{1/6} = \frac{1}{6} \]

(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) \( P(A|B) \)

There are 3 ways to get exactly 2 heads (event \( B \)) HHT HTH THH. Two of these make \( A \) true, so \( P(A|B) = \frac{2}{3} \).

(2) \( P(B|A) \)

There are 4 possible results given \( A \) HHH HTH HHT HTT. Two of these give event \( B \) so \( P(B|A) = \frac{1}{2} \).

(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?

The three coins have 6 faces so the total number outcomes is \( N = 6 \). Let \( D \) be the event that the coin is double-headed and \( A \) be the event that it shows a head. Then 3 faces yield \( A \), so \( P(A) = \frac{1}{2} \). Two faces yield \( A \) and \( D \) (as it can be either way up) so \( P(A \land D) = \frac{1}{3} \). Finally,

\[ P(D|A) = \frac{P(A \land D)}{P(A)} = \frac{2}{3} \]
The point is that many people are prepared to argue as follows:

If the coin shows a head, it is either double-headed or the conventional coin. Since the coin was picked at random, these are equally likely, so 

\[ P(D|A) = \frac{1}{2}. \]

This is superficially plausible, but as we have seen it is totally wrong.

(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?

Let \( B \) be the event that the first sock is blue and \( A \) the event that you have a pair of blue socks. If you have one blue sock, the probability that the second is blue is the chance of drawing one of the 2 remaining blues from the 7 remaining socks. That is to say \( P(A|B) = \frac{2}{7} \). Here \( A = A \land B \) and so

\[ P(A) = P(A \land B) = P(A|B)P(B) = \frac{2}{7} \times \frac{3}{8} = \frac{3}{28}. \]

(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?

Let \( A \) be the event that you buy a genuine article and let \( D \) be the event that your purchase is defective. We know that

\[ P(A) = \frac{9}{10}, \quad P(\sim A) = \frac{1}{10}, \quad P(D|A) = \frac{1}{1000}, \quad P(D|\sim A) = \frac{1}{2}. \]

Hence we have

\[ P(D) = P(D|A)P(A) + P(D|\sim A)P(\sim A) = \frac{9}{10000} + \frac{1}{20} \approx 0.05. \]

(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?

Let \( B \) be the event that no side effects occur. We are given that

\[ P(A|B \land C) = \frac{99}{100}, \quad P(B|C) = \frac{95}{100}, \quad P(\sim A|B \land C) = \frac{5}{100}, \quad P(\sim B|C) = \frac{5}{100}. \]

Therefore,

\[ P(A|C) = P(A|B \land C)P(B|C) + P(\sim A|B \land C)P(\sim B|C) \]

\[ = \frac{99}{100} \times \frac{95}{100} + \frac{5}{100} \times \frac{5}{100} \times \frac{9555}{10000} = 0.9555. \]
(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?

Let $A$ be the event that the question is answered correctly and $S$ the event that the student knew the answer. We require $P(S|A)$. To use Bayes’ rule, we need to calculate $P(A)$, thus

$$P(A) = P(A|S)P(S) + P(A|\sim S)P(\sim S) = (1)p + \left(\frac{1}{c}\right)(1-p) = p + \left(\frac{1}{c}\right)(1-p)$$

Therefore,

$$P(S|A) = \frac{P(A|S)P(S)}{P(A)} = \frac{p}{p + \left(\frac{1}{c}\right)(1-p)} = \frac{cp}{1 + (c-1)p}$$

Notice that the larger $c$ is, the more likely it is that the student knew the answer to the question (given that it is answered correctly).

(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?

The total number of possibilities is $N = 9 \times 10 \times 10 \times 10 = 9000$. If $A$ is the event that no digit is repeated, then $N_A = 9 \times 9 \times 8 \times 7 = 4536$. Thus,

$$P(A) = \frac{N_A}{N} = \frac{4536}{9000} = 0.504$$

(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?

First we note the number of possibilities is given by all possible choices of 5 cards from 52 cards or

$$N = \binom{52}{5} = \frac{52!}{5!47!} = \frac{52 \times 51 \times 50 \times 49 \times 48}{1 \times 2 \times 3 \times 4 \times 5} = 2598960$$

For a full house you can choose the value of the triple in 13 ways and then you can choose their three suits in

$$\binom{4}{3}$$

ways. The value of the double can then be chosen in 12 ways and their suits in

$$\binom{4}{2}$$

ways. The value of the double can then be chosen in 12 ways and their suits in

$$\binom{4}{2}$$
ways. Hence

$$P(\text{full house}) = \frac{13 \left( \begin{array}{c} 4 \\ 3 \end{array} \right) 12 \left( \begin{array}{c} 4 \\ 2 \end{array} \right)}{N} = \frac{3744}{2598960} = 1.441 \times 10^{-3}$$

For 4 of a kind, we can choose 13 different sets and their 4 different suits in

$$\left( \begin{array}{c} 4 \\ 4 \end{array} \right) = 1$$

ways. The last card can then be chosen in 48 ways so that we have

$$\frac{48 \times 13}{2598960} = 2.4 \times 10^{-4}$$
as the probability.

### 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).

Let $S =$ *spade* and $N =$ *not spade*. Then the symbol $N_1 S_2 S_3$ means: 1st card drawn is not a spade, 2nd card drawn is a spade, 3rd card drawn is a spade. In this notation, the possible ways of discarding 2 cards and then drawing a spade are:

$$S_1 S_2 S_3, \quad S_1 N_2 S_3, \quad N_1 S_2 S_3, \quad N_1 N_2 S_3$$

These events are mutually exclusive, therefore using

$$P(A \lor B) = P(A) + P(B)$$
i.e., we add their probabilities. Now to compute the probability of, say, $S_1 N_2 S_3$, we use the equation $P(A \land B) = P(A)P(B)$ repeatedly. The probability of $S_1$ is $13/52$. Then the probability of $N_2$ is $39/51$ since there are now 51 cards left and 39 of them are not spades. Now the probability of $S_3$ is $12/50$ since there are 12 spades left and 50 cards left. Thus

$$P(S_1 N_2 S_3) = \frac{13}{52} \times \frac{39}{51} \times \frac{12}{50}$$

Similarly,

$$P(S_1 S_2 S_3) = \frac{13}{52} \times \frac{12}{51} \times \frac{11}{50}$$
$$P(N_1 S_2 S_3) = \frac{39}{52} \times \frac{12}{51} \times \frac{11}{50}$$
$$P(N_1 N_2 S_3) = \frac{39}{52} \times \frac{38}{51} \times \frac{13}{50}$$

which gives

$$P(3^{rd} \text{ card is a spade}) = P(S_1 N_2 S_3) + P(S_1 S_2 S_3) + P(N_1 S_2 S_3) + P(N_1 N_2 S_3)$$

$$= \frac{13}{52} \left[ \frac{12(11+39)+39(12+38)}{51 \times 50} \right] = \frac{1}{4}$$
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 \( n \ll 365 \) by calculating \( \log(p) \) (use the fact that \( \log(1+x) \approx x \) for \( x \ll 1 \)). Find the smallest integer \( N \) for which \( p < \frac{1}{2} \). Hence show that for a group of \( N \) people or more, the probability is greater than \( \frac{1}{2} \) that two of them have the same birthday.

The probability that 2 people have different birthdays is the probability that the 2\(^{nd} \) person was born on one of the 364 other than the birthday of the first person; this probability = \( \frac{364}{365} \). The probability that the 3\(^{rd} \) person has a different birthday from either of the first two is = \( \frac{363}{365} \), and so on. Now using the equation \( P(A \cap B) = P(A)P(B) \) the probability that the first two people have different birthdays and then that the third person has a still different birthday is the product

\[
P(A \cap B) = \frac{364}{365} \times \frac{363}{365} = \left(1 - \frac{1}{365}\right) \left(1 - \frac{2}{365}\right)
\]

Continuing in this way for \( n \) people, we have

\[
p = P(\text{all different birthdays}) = \left(1 - \frac{1}{365}\right) \left(1 - \frac{2}{365}\right) \ldots \left(1 - \frac{n-1}{365}\right)
\]

Now

\[
\ln(p) = \ln \left(1 - \frac{1}{365}\right) + \ln \left(1 - \frac{2}{365}\right) + \ldots + \ln \left(1 - \frac{n-1}{365}\right)
\]

and

\[
\ln (1 - x) \approx -x \quad \text{for} \quad x \ll 1
\]

Thus, for \( (n-1) \ll 365 \) we have

\[
\ln(p) = -\frac{1}{365} - \frac{2}{365} - \ldots - \frac{n-1}{365} = -\frac{1+2+\ldots+(n-1)}{365} = -\frac{n(n-1)}{2 \times 365}
\]

If \( p < \frac{1}{2} \) or \( \ln(p) < \ln(\frac{1}{2}) = -\ln(2) \), then we want

\[
-\ln(2) > -\frac{n(n-1)}{2 \times 365} \Rightarrow \frac{n(n-1)}{2 \times 365} > \ln(2) \Rightarrow n \geq 23
\]

Thus, in a group of 23 people, the probability is slightly over \( \frac{1}{2} \) that two people will have the same birthday. For 50 people, the probability of coincidence is about 0.97
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)?

The probability of life in the vicinity of some arbitrarily selected star is equal to \( pqr = 10^{-6} \), assuming that the three conditions are independent.

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

The probability \( P \) that life exists in the vicinity of at least one star is given by \( P = 1 - P_0 \), where \( P_0 \) is the probability that no stars have life about them.

The probability of no life about some arbitrarily selected star is \( 1 - pqr \). Therefore, we have

\[
P_0 = (1 - pqr)^N
\]

Now

\[
\log P_0 = N \log(1 - pqr) \approx N(-pqr) = -10^5
\]

so that

\[
P_0 = e^{-pqrN} \approx e^{-10^5} \approx 0
\]

Thus,

\[
P = 1 - P_0 \approx 1
\]

This says that even a very rare event is almost certain to occur in a large enough sample.

NOTE: A naive argument against a purely natural origin of life is sometimes based on the smallness of the probability (a), whereas it is the probability (b) that is relevant!

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?
The binomial formula for the probability of \( n_H \) heads in \( n \) trials is

\[
P(n_H|M^n) = \frac{n!}{n_H!(n-n_H)!} \left( \frac{1}{2} \right)^n \text{ for } p = q = \frac{1}{2}
\]

If we define

\[
\text{binomial}(k,n,p) = \text{probability}(x \geq k) = \sum_{x=k}^{n} \frac{n!}{x!(n-x)!} p^x (1-p)^{n-x}
\]

then

\[
P(n_H|M^n) = \text{binomial}(n_H,n,0.5) - \text{binomial}(n_H+1,n,0.5)
\]

and

\[
P(m \leq n_H \leq s|M^n) = \text{binomial}(m,n,0.5) - \text{binomial}(s+1,n,0.5)
\]

**Exactly 1/2 heads:**

\[
P(5|M^{10}) = 0.246 , \quad P(50|M^{100}) = 0.0796
\]
\[
P(500|M^{1000}) = 0.0252 , \quad P(5000|M^{10000}) = 0.00798
\]

which clearly approaches zero as it should.

**In range:**

\[
P(4.45 \leq n_H \leq 5.55|M^{10}) = 0.246 , \quad P(44.5 \leq n_H \leq 55.5|M^{100}) = 0.7288
\]
\[
P(445 \leq n_H \leq 555|M^{1000}) = 0.999552 , \quad P(4450 \leq n_H \leq 5550|M^{10000}) = 1.0000
\]

so that

\[
P(\text{exactly 1/2}) \to 0 \text{ as } N \to \infty
\]

but

\[
P(\text{to be in vicinity of 1/2}) \to 1 \text{ as } N \to \infty
\]

### 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.

Let \( A \) mean *nickel* and \( B \) mean *right pocket*. Then we want the conditional probability \( P(B|A) \). We use Bayes’ formula

\[
P(B|A) = \frac{P(A|B)P(B)}{P(A)}
\]
Now $P(A|B)P(B) = \text{probability of selecting the right pocket and then selecting a nickel from it. Thus,}$

\[
P(B) = P(\text{right pocket}) = \frac{1}{2} \text{ (two equally likely pockets)}
\]

\[
P(A|B) = P(\text{nickel|right pocket}) = \frac{3}{7} \text{ (3 nickels out of 7 coins)}
\]

\[
P(A|B)P(B) = \frac{1}{2} \times \frac{3}{7} = \frac{3}{14}
\]

Now

\[
P(A) = P(\text{nickel}) = P(\text{nickel|right})P(\text{right}) + P(\text{nickel|left})P(\text{left})
\]

\[
= P(A|B)P(B) + P(A|\sim B)P(\sim B)
\]

\[
= \frac{3}{7} \times \frac{1}{2} + \frac{2}{7} \times \frac{1}{2} = \frac{5}{14}
\]

Therefore, the probability that the nickel came from the right pocket is

\[
P(B|A) = \frac{P(A|B)P(B)}{P(A)} = \frac{3/14}{23/42} = \frac{9}{23}
\]

5.6.7 Psychological Tests

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

$I = \text{In a certain city, 85% of the taxicabs are blue and 15% are green}$

and the data:

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

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

Let $B = \text{event that taxicab was actually blue. From Bayes’ theorem, the correct answer is}$

\[
P(B|D \land I) = \frac{P(D|B \land I)P(B)}{P(D)} = \frac{(0.2) \times (0.85)}{(0.2) \times (0.85) + (0.8) \times (0.15)} = \frac{17}{27} = 0.63
\]

This is easiest to reason out in one’s head using odds; since the statement of the problem told us that the witness was equally likely to err in either direction ($G \rightarrow B$ or $B \rightarrow G$), Bayes’ theorem reduces to simple multiplication of odds. The prior odds in favor of blue are 85 : 15, or nearly 6 : 1; but the odds on
the witness being right are only $80 : 20 = 4 : 1$, so the posterior odds on blue are $85 : 60 = 17 : 12$. Yet most people tend to guess $P(B|D \land I)$ as about 0.2, corresponding to the odds of 4 : 1 in favor of green, thus ignoring the prior information. For these guesses, the data come first with a vengeance, even though the prior information implies many more observations than the single datum.

The opposite error - clinging irrationally to prior opinions in the face of massive contrary evidence - is equally familiar to us that is the stuff of which fundamentalist religious/political stances are made. In general, the intuitive force of prior opinions depends on how long we have held them.

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,

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

Our measuring device is not perfect. Due to noise it can only measure with a resolution $\Delta$, 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,

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

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

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

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?

We are trying to determine the position of a particle along one dimension. Our prior probability distribution is a Gaussian

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

which looks like
We now measure the position and find the value $y$ in my detector. However, my detector has only finite resolution, so when my detector reads "$y$", the true position "$x$" may still be different. Given an uncertainty $\Delta x$ in my detector with a Gaussian distribution, let the likelihood distribution be

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

Thus, according to Bayes’ rule, the updated probability assignment is

$$P(x|y) = NP(y|x)P(x)$$

where

$$N^{-1} = \int dxP(y|x)P(x)$$

is a normalization factor.

Let us first calculate

$$P(y|x)P(x) = \frac{1}{2\pi\sigma_0 \Delta} e^{-\frac{(x-x_0)^2}{2\sigma_0^2} - \frac{(y-x)^2}{2\Delta^2}}$$

Aside:

$$\frac{(x-x_0)^2}{\sigma_0^2} + \frac{(y-x)^2}{\Delta^2} = \frac{x^2 - 2xx_0 + x_0^2}{\sigma_0^2} + \frac{x^2 - 2xy + y^2}{\Delta^2} = \frac{x^2}{\sigma^2} - 2x\left(\frac{x_0}{\sigma_0^2} + \frac{y}{\Delta^2}\right) + \frac{x_0^2}{\sigma_0^2} + \frac{y^2}{\Delta^2} = \frac{x^2}{\sigma^2} - 2xA(y) + B(y)$$

where

$$\frac{1}{\sigma^2} = \frac{1}{\sigma_0^2} + \frac{1}{\Delta^2} \; , \; A(y) = \frac{x_0}{\sigma_0^2} + \frac{y}{\Delta^2} \; , \; B(y) = \frac{x_0^2}{\sigma_0^2} + \frac{y^2}{\Delta^2}$$

Trick: Complete the square.

$$\frac{x^2}{\sigma^2} - 2xA(y) = \frac{(x-x')^2}{\sigma^2} - \frac{x'^2}{\sigma^2}$$
where

\[ x' = \sigma'^2 A(y) = \left( \frac{x_0}{\sigma_0^2} + \frac{y}{\Delta^2} \right) \sigma'^2 \]

or

\[ x' = x_0 + x_0 \left( 1 - \frac{\sigma'^2}{\sigma_0^2} \right) + \frac{y \sigma'^2}{\Delta^2} \]

Now

\[ \sigma'^2 = \frac{\sigma_0^2 \Delta^2}{\sigma_0^2 + \Delta^2} \]

which implies that

\[ x' = x_0 + K_1 (y - x_0) \]

where

\[ K_1 = \frac{\sigma_0^2}{\sigma_0^2 + \Delta^2} \]

Putting this all together we have

\[ P(y|x) P(x) = N(y, x_0) e^{-\frac{(x-x')^2}{2\sigma'^2}} \]

where \( N(y, x_0) \) contains all the rest of the factors. Instead of keeping track of all of these factors we can just replace it by the correct normalization

\[ P(x|y) = \frac{1}{\sqrt{2\pi\sigma'^2}} e^{-\frac{(x-x')^2}{2\sigma'^2}} \]

where

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

Graphically we have
After the measurement, the new distribution is a narrower Gaussian peaked closer to the actual position. That is called Bayes’ learning.

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:

<table>
<thead>
<tr>
<th>Item</th>
<th>Entree</th>
<th>Cost</th>
<th>Calories</th>
<th>Prob(hot)</th>
<th>Prob(cold)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Meal 1</td>
<td>burger</td>
<td>$1.00</td>
<td>1000</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Meal 2</td>
<td>chicken</td>
<td>$2.00</td>
<td>600</td>
<td>0.8</td>
<td>0.2</td>
</tr>
<tr>
<td>Meal 3</td>
<td>fish</td>
<td>$3.00</td>
<td>400</td>
<td>0.9</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 5.1: Berger’s Burgers Details

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

\[ \text{Prob(burger)} = P(B) \]
\[ \text{Prob(chicken)} = P(C) \]
\[ \text{Prob(fish)} = P(F) \]

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

\[ 1 = \sum_i P(A_i) \] (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

\[ S = \sum_i P(A_i) \log_2 \left( \frac{1}{P(A_i)} \right) \] (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.

Constraints take the form

\[ G = \text{expected value} = \sum_i P(A_i)g(A_i) \]

We have the constraints

\[ 1 = P(B) + P(C) + P(F) \]
\[ 1.75 = 1.00P(B) + 2.00P(C) + 3.00P(F) \]

Since we have 3 unknowns and only 2 equations, there is not enough information to solve for the unknowns. The amount of our uncertainty about the probability distribution is the entropy, which is given by

\[ S = P(B)\log_2 \left( \frac{1}{P(B)} \right) + P(C)\log_2 \left( \frac{1}{P(C)} \right) + P(F)\log_2 \left( \frac{1}{P(F)} \right) \]

What should our strategy be? There are a range of values of the probabilities that are consistent with this information set. Each solution, however,
leaves us with different amounts of uncertainty $S$. If we choose a solution for which $S$ is small, we are assuming something that we do not know. For example, if our average had been 2.00 instead of 1.75, then we could meet both constraints by assuming that everybody bought the chicken meal. The our solution would be\[ P(B) = P(F) = 0 \text{ and } P(C) = 1 \]
which corresponds to an uncertainty of 0 bits. Or we could assume that half the orders are for burgers and half for fish. In this case the solution would be\[ P(B) = P(F) = 1/2 \text{ and } P(C) = 0 \]
which corresponds to an uncertainty of 1 bit.

Neither of these assumptions seems appropriate because each goes beyond what we know.

The only way to find the probability distribution that uses no further assumptions beyond what we already know is to use the MaxEnt principle. This principle state that we select the probability distribution that gives the largest uncertainty (maximum entropy) consistent with the constraints. In this way, we are not introducing any additional assumptions or biases into the calculations.

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

\[
\begin{align*}
a &\leq P(B) \leq b \\
c &\leq P(C) \leq d \\
e &\leq P(F) \leq f
\end{align*}
\]

For this case we can solve the problem analytically. We can express, using the constraint equation, two of the unknown probabilities in terms of the third. We have

\[
\begin{align*}
P(C) &= 0.75 - 2P(F) \\
P(B) &= 0.25 + P(F)
\end{align*}
\]

Since each of the probabilities lies between 0 and 1, it is clear that

\[
0P(F)0.375 \text{ (expected value constraint)} \\
0P(C)0.75 \text{ (last equations)} \\
0.25P(B)0.625 \text{ (last equations)}
\]
or

\[
\begin{align*}
0.0 &\leq P(F) \leq 0.375 \\
0.0 &\leq P(C) \leq 0.75 \\
0.25 &\leq P(B) \leq 0.625
\end{align*}
\]
(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 \(S\).

The entropy then becomes

\[
S = \left(0.25 + P(F)\right) \log_2 \left(\frac{1}{0.25 + P(F)}\right) + \left(0.75 - 2P(F)\right) \log_2 \left(\frac{1}{0.75 - 2P(F)}\right) + P(F) \log_2 \left(\frac{1}{P(F)}\right)
\]

The maximum occurs for \(P(F) = 0.216\) and hence for \(P(B) = 0.466\) and \(P(C) = 0.318\) and \(S = 1.517\) bits.

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

Average Calorie Count = \(1000P(B) + 600P(C) + 400P(F)\)

\[
= 466.0 + 190.8 + 86.4 = 743.2
\]

Average Meals Cold = \(0.5P(B) + 0.2P(C) + 0.1P(F)\)

\[
= 0.233 + 0.064 + 0.022 = 0.319
\]

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:

<table>
<thead>
<tr>
<th>Entree</th>
<th>Cost</th>
<th>Calories</th>
<th>Prob(hot)</th>
<th>Prob(cold)</th>
</tr>
</thead>
<tbody>
<tr>
<td>burger</td>
<td>$1.00</td>
<td>1000</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>chicken</td>
<td>$2.00</td>
<td>600</td>
<td>0.8</td>
<td>0.2</td>
</tr>
<tr>
<td>fish</td>
<td>$3.00</td>
<td>400</td>
<td>0.9</td>
<td>0.1</td>
</tr>
<tr>
<td>tofu</td>
<td>$8.00</td>
<td>200</td>
<td>0.6</td>
<td>0.4</td>
</tr>
</tbody>
</table>

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.

We now have the constraints
\[
1 = P(B) + P(C) + P(F) + P(T)
\]
\[
2.50 = 1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(T)
\]
and the entropy function
\[
S = P(B) \log_2 \left( \frac{1}{P(B)} \right) + P(C) \log_2 \left( \frac{1}{P(C)} \right) + P(F) \log_2 \left( \frac{1}{P(F)} \right) + P(T) \log_2 \left( \frac{1}{P(T)} \right)
\]

The analytical method used in problem 5.6.9 will not work in this problem where there are 4 probabilities and only 1 constraint equation. We have 4 unknowns and only 2 equations so that the entropy would be a function of two variables and thus finding the maximum would require gradient search techniques.

The more general procedure in this case uses Lagrange multipliers. We define the Lagrange multipliers \(\alpha\) and \(\beta\) and then the Lagrangian function \(L\):
\[
L = S - (\alpha - \log_2 e)(P(B) + P(C) + P(F) + P(T) - 1) - \beta(1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(T) - 2.50)
\]

The reason for the addition of the term \(\log_2 e\) will be clear shortly.

Maximizing \(L\) with respect to each of the probabilities is done by differentiating \(L\) with respect to each probability while keeping \(\alpha\) and \(\beta\) and all the other probabilities constant. The results are
\[
\frac{\partial L}{\partial P(B)} = 0 = \frac{\partial S}{\partial P(B)} - (\alpha - \log_2 e) - \beta = \log_2 \left( \frac{1}{P(B)} \right) - \log_2 e - (\alpha - \log_2 e) - \beta \\
\log_2 \left( \frac{1}{P(B)} \right) = \alpha + \beta
\]

and similarly
\[
\log_2 \left( \frac{1}{P(C)} \right) = \alpha + 2\beta , \quad \log_2 \left( \frac{1}{P(F)} \right) = \alpha + 3\beta , \quad \log_2 \left( \frac{1}{P(T)} \right) = \alpha + 8\beta
\]

so that
\[
P(B) = 2^{-\alpha}2^{-\beta} \\
P(C) = 2^{-\alpha}2^{-2\beta} \\
P(F) = 2^{-\alpha}2^{-3\beta} \\
P(T) = 2^{-\alpha}2^{-8\beta}
\]

We can find \(\alpha\) and \(\beta\) using
\[
P(B) + P(C) + P(F) + P(T) = 1 \\
2^{-\alpha}(2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta}) = 1 \\
\log_2 \left( 2^{-\alpha}(2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta}) \right) = 0 \\
\alpha = \log_2 \left( 2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta} \right)
\]
and

\[
2^\alpha (1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(T)) = 2.50 \times 2^\alpha \\
1 \times 2^{-\beta} + 2 \times 2^{-2\beta} + 3 \times 2^{-3\beta} + 8 \times 2^{-8\beta} = 2.50 \times 2^\alpha \\
1 \times 2^{-\beta} + 2 \times 2^{-2\beta} + 3 \times 2^{-3\beta} + 8 \times 2^{-8\beta} = 2.50 \times (2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta}) \\
1.50 \times 2^{-\beta} + 0.50 \times 2^{-2\beta} - 0.50 \times 2^{-8\beta} = 0
\]

Finding the zeroes of the last equation gives us \( \beta \) and the value of \( \beta \) gives us \( \alpha \), which then determine the probabilities and the entropy. The computed values are

\[
\beta = 0.2586 \text{ bits/dollar} \\
\alpha = 1.2371 \text{ bits} \\
P(B) = 0.3546 \\
P(C) = 0.2964 \\
P(F) = 0.2478 \\
P(T) = 0.1011 \\
S = 1.8835 \text{ bits}
\]

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 \( t \), \( P(n,t) \).

We have random arrival at the detector with an average rate \( R \). Consider breaking up any time interval into slices of size \( \Delta t \) such that no more than one particle arrives in that interval. The probability for a particle to be in the interval \( \Delta t \) is

\[
P_{\Delta t} = R\Delta t \ll 1
\]

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

Now consider a finite interval from 0 to \( t \). There are \( N = t/\Delta t \) slices in the interval. Let \( q_{\Delta t} = 1 - P_{\Delta t} \) probability of no particle in the slice.

Since the different slices are statistically independent, this implies that the probability of no detection in the interval \([0,t]\) is given by

\[
(q_{\Delta t})^N = (1 - P_{\Delta t})^N = (1 - R\Delta t)^{t/\Delta t}
\]
This implies that

\[ P(0, t) = \lim_{\Delta t \to 0} (1 - R\Delta t)^{t/\Delta t} = e^{-Rt} \]

(b) Obtain a differential equation as a recursion relation

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

Now, in the interval \( t \to t + \Delta t \) either no particles or one particle is detected. This implies that

\[ P(n, t + \Delta t) = P(n, t)P(0, \Delta t) + P(n - 1, t)P(1, \Delta t) = P(n, t)(1 - R\Delta t) + P(n - 1, t)(R\Delta t) \]

Therefore,

\[ \frac{d}{dt} P(n, t) = \lim_{\Delta t \to 0} \frac{P(n, t + \Delta t) - P(n, t)}{\Delta t} = R(P(n - 1, t) - P(n, t)) \]

(c) Solve this to find the Poisson distribution

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

Plot a histogram for \( Rt = 0.1, 1.0, 10.0 \).

We can solve this recursively.

\[ \frac{d}{dt} P(0, t) = -RP(0, t) \to P(0, t) = e^{-Rt} \]

\[ \frac{d}{dt} P(1, t) = R(P(0, t) - P(1, t)) = -RP(1, t) + e^{-Rt} \]

With initial condition \( P(1, t = 0) = 0 \), this implies that

\[ P(1, t) = Rte^{-Rt} \]

\[ \frac{d}{dt} P(2, t) = R(P(1, t) - P(2, t)) = -RP(2, t) + Rte^{-Rt} \to P(2, t) = \frac{1}{2} (Rt)^2 e^{-Rt} \]

By induction we have

\[ P(n, t) = \frac{1}{n!} (Rt)^n e^{-Rt} \]
Figure 5.1: \( R_t = 0.1 \)
Figure 5.2: $R_t = 1.0$
Figure 5.3: $R_t = 10.0$
Note that as $Rt \to \infty$ we get a Gaussian (this is the central limit theorem).

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

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

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

The expected value is

$$\langle n \rangle = \sum_{n=0}^{\infty} n P(n, t) = \sum_{n=0}^{\infty} \frac{n}{n!} (Rt)^n e^{-Rt}$$

$$= \left( \sum_{n=0}^{\infty} \frac{1}{(n-1)!} (Rt)^n \right) e^{-Rt} = \left( \sum_{m=0}^{\infty} \frac{1}{m!} (Rt)^{m+1} \right) e^{-Rt}$$

$$= Rt \left( \sum_{m=0}^{\infty} \frac{1}{m!} (Rt)^m \right) e^{-Rt} = Rt (e^{Rt}) e^{-Rt} = Rt$$

Now

$$\sigma_n^2 = \langle n^2 \rangle - \langle n \rangle^2$$

**Trick:** Consider

$$\langle n^2 \rangle - \langle n \rangle = \langle n(n-1) \rangle = \sum_{n=0}^{\infty} \frac{(Rt)^n}{(n-2)!} e^{-Rt}$$

as in equations above. Thus,

$$\sigma_n^2 = \langle n(n-1) \rangle + \langle n \rangle - \langle n \rangle^2$$

$$= (Rt)^2 t - (Rt)^2 = Rt \to \sigma_n = \sqrt{\langle n \rangle}$$

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.

The Poisson distribution can be seen as the limit of a Binomial distribution. In the interval $[0, t]$ with $N = t/\Delta t$ intervals we seek the probability for $n$ counts. In the Binomial case we have

$$P(N, n) = \binom{N}{n} p^n (1 - p)^{N-n}$$
The probability of "heads" = a count in $\Delta t$: $p = R \Delta t = Rt/N$ which implies that

$$P(N,n) = \frac{N!}{n!(N-n)!} \left( \frac{Rt}{N} \right)^n \left( \frac{1 - \frac{Rt}{N}}{1 - \frac{Rt}{N}} \right)^n$$

Now, take the limit as $N \to \infty$ with $Np = Rt = \text{finite}$ and using the fact that

$$\lim_{N \to \infty} \left( 1 - \frac{Rt}{N} \right)^N = e^{-Rt}, \quad \lim_{N \to \infty} \left( 1 - \frac{Rt}{N} \right)^n = 1$$

and

$$\lim_{N \to \infty} \frac{N!}{(N-n)!} \left( \frac{Rt}{N} \right)^n = \lim_{N \to \infty} (Rt)^n(1-1/N)(1-2/N)\cdots(1-(n-1)/N) = (Rt)^n$$

to get

$$\lim_{N \to \infty} P(N,n) = \frac{(Rt)^n}{n!} e^{-Rt}$$

which is 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

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

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 $b$:

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

\[
\langle s \rangle = \sum_{i=2}^{12} i \Pr(s = i)
\]

and

\[
\langle p \rangle = \sum_{i=1}^{36} i \Pr(p = i).
\]

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?

The minimum possible value of \( s \) is 2 and its maximum possible value is 12. By straightforward and tedious calculation we then have

\[
\langle s \rangle = 2 \Pr(a = 1) \Pr(b = 1) + 3(\Pr(a = 1) \Pr(b = 2) + \Pr(a = 2) \Pr(b = 1))
+ 4[\Pr(a = 3) \Pr(b = 1) + \Pr(a = 2) \Pr(b = 2) + \Pr(a = 1) \Pr(b = 3)]
+ 5[\Pr(a = 4) \Pr(b = 1) + \Pr(a = 3) \Pr(b = 2) + \Pr(a = 2) \Pr(b = 3)
+ \Pr(a = 1) \Pr(b = 4)]
+ 6[\Pr(a = 5) \Pr(b = 1) + \Pr(a = 4) \Pr(b = 2) + \Pr(a = 3) \Pr(b = 3)
+ \Pr(a = 2) \Pr(b = 4) + \Pr(a = 1) \Pr(b = 5)]
+ 7[\Pr(a = 6) \Pr(b = 1) + \Pr(a = 5) \Pr(b = 2) + \Pr(a = 4) \Pr(b = 3)
+ \Pr(a = 3) \Pr(b = 4) + \Pr(a = 2) \Pr(b = 5) + \Pr(a = 1) \Pr(b = 6)]
+ 8[\Pr(a = 6) \Pr(b = 2) + \Pr(a = 5) \Pr(b = 3) + \Pr(a = 4) \Pr(b = 4)
+ \Pr(a = 3) \Pr(b = 5) + \Pr(a = 2) \Pr(b = 6)]
+ 9[\Pr(a = 6) \Pr(b = 3) + \Pr(a = 5) \Pr(b = 4) + \Pr(a = 4) \Pr(b = 5)
+ \Pr(a = 3) \Pr(b = 6)]
+ 10[\Pr(a = 6) \Pr(b = 4) + \Pr(a = 5) \Pr(b = 5) + \Pr(a = 4) \Pr(b = 6)]
+ 11[\Pr(a = 6) \Pr(b = 5) + \Pr(a = 5) \Pr(b = 6)]
+ 12\Pr(a = 6) \Pr(b = 6)
= \frac{1}{36} \cdot 252 = 7
\]

Since \( \langle a \rangle = \langle b \rangle = 7/2 \), we have \( \langle s \rangle = \langle a \rangle + \langle b \rangle \). This has to be the case since expectation is linear.

Likewise, for \( p \), the minimum value is 1 and the maximum value is 36. In table form,
and thus,

\[ \langle p \rangle = \frac{1}{36} \left[ 1 + 2(2) + 3(2) + 4(3) + 5(2) + 6(4) + 8(2) + 9 + 10(2) + 12(4) + 15(2) + 16 + 18(2) + 20(2) + 24(2) + 25 + 30(2) + 36 \right] \]

\[ = \frac{1}{36} \left[ 1 + 4 + 6 + 12 + 10 + 24 + 16 + 9 + 20 + 48 + 30 + 16 + 36 + 40 + 48 + 25 + 60 + 36 \right] \]

\[ = \frac{441}{36} = 12.25 \]

Since \( \langle a \rangle \langle b \rangle = 49/4 = 12.25 \), we have \( \langle ab \rangle = \langle a \rangle \langle b \rangle \). This reflects the fact that \( a \) and \( b \) are statistically independent (uncorrelated).

### 5.6.13 Conditional Probabilities for Dice

Use the results of Problem 5.6.12. 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 \( a \)?

If \( s = 8 \), then the only possible die combinations are (2, 6)(3, 5)(4, 4)(5, 3)(6, 2). Hence, the forward conditional probability distribution \( Pr(s = 8|a = i) \) for \( a \) is \([0, 1/6, 1/6, 1/6, 1/6, 1/6, 1/6] \). Via Bayes’ rule,

\[ Pr(a = i|s = 8) = \frac{Pr(s = 8|a = i)Pr(a = i)}{Pr(s = 8)} = \frac{Pr(s = 8|a = i)\frac{1}{5}}{\frac{5}{36}} \]

\[ = Pr(s = 8|a = i)\frac{6}{5} \]

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The forward conditional probabilities are then

\[ Pr(s = 8|a = 1) = 0 \]
\[ Pr(s = 8|a = 2) = Pr(b = 6) = \frac{1}{6} \]
\[ Pr(s = 8|a = 3) = Pr(b = 5) = \frac{1}{6} \]
\[ Pr(s = 8|a = 4) = Pr(b = 4) = \frac{1}{6} \]
\[ Pr(s = 8|a = 5) = Pr(b = 3) = \frac{1}{6} \]
\[ Pr(s = 8|a = 6) = Pr(b = 2) = \frac{1}{6} \]

(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 \( s \)?

If \( p = 12 \), then the possible combinations \((a, b)\) are \((2, 6)(3, 4)(4, 3)(6, 2)\). Hence, the conditioned probability distribution for \( s \) is \( Pr(s = 7) = Pr(s = 8) = 1/2 \) and the conditioned expectation value is 15/2.

### 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

\[ x_0 = \left( \frac{\sqrt{p_h}}{\sqrt{p_t}} \right) \]

(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

\[ x_0^T Rx_0 = \langle r \rangle \]

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

We have

\[ R = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

\[ x_0^T Rx_0 = \left( \frac{\sqrt{p_h}}{\sqrt{p_t}} \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \sqrt{p_h} \\ \sqrt{p_t} \end{pmatrix} \]

\[ = \left( \frac{\sqrt{p_h}}{\sqrt{p_t}} \right) \begin{pmatrix} \sqrt{p_h} \\ -\sqrt{p_t} \end{pmatrix} \]

\[ = p_h - p_t \]
(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

$$x_0 \mapsto Fx_0$$

and

$$\langle r \rangle \mapsto x_0^T F^T RFx_0$$

Does $U = F^T RF$ 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 $F^T R$?

We have

$$F = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Fx_0 = \begin{pmatrix} \sqrt{p_t} \\ \sqrt{p_h} \end{pmatrix}$$

$$F^T RF = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$x_0^T F^T RFx_0 = -p_h + p_t$$

Obviously, $F^T RF$ is just the observable that takes value $-1$ for heads and $+1$ for tails. On the other hand

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

$$x_0^T RFx_0 = \begin{pmatrix} \sqrt{p_h} & \sqrt{p_t} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{p_h} \\ \sqrt{p_t} \end{pmatrix} = \sqrt{p_h}p_t - \sqrt{p_h}p_t$$

which vanishes for any coin! So it can only be interpreted as a trivial (constant with value 0) observable. Likewise

$$F^T R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$x_0^T F^T Fx_0 = \begin{pmatrix} \sqrt{p_h} & \sqrt{p_t} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{p_h} \\ \sqrt{p_t} \end{pmatrix} = -\sqrt{p_h}p_t + \sqrt{p_h}p_t$$

which also vanishes.

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

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

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

$$v_1, v_2 \in V, \quad v_1v_2 = v_2v_1$$

Is $U$ in this set? How should we interpret the observable represented by an arbitrary element $v \in V$?
We have
\[ aR + bR^2 = \begin{pmatrix} a + b & 0 \\ 0 & b - a \end{pmatrix} \]

By varying \( a \) and \( b \), we can thus generate any matrix of the form
\[ v = \begin{pmatrix} c & 0 \\ 0 & d \end{pmatrix} \]

where \( c \) and \( d \) are arbitrary real numbers. Likewise all elements of \( V \) are of this form. Hence,
\[ v_1v_2 = \begin{pmatrix} c_1 & 0 \\ 0 & d_1 \end{pmatrix} \begin{pmatrix} c_2 & 0 \\ 0 & d_2 \end{pmatrix} = \begin{pmatrix} c_1c_2 & 0 \\ 0 & d_1d_2 \end{pmatrix} \]

which is still in \( V \), and clearly \( v_1v_2 = v_2v_1 \). We get \( U \) by setting \((a, b) = (-1, 0)\), and in general we interpret \( v \) as the observable that takes value \( c \) for heads and \( d \) for tails.
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,

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

First assume $\hat{\rho}$ represents a state vector which implies that

$$\hat{\rho} = \hat{P}|\psi\rangle = |\psi\rangle \langle \psi|$$

for some normalized state $|\psi\rangle$. Then

$$\hat{\rho}^2 = (|\psi\rangle \langle \psi|)(|\psi\rangle \langle \psi|) = |\psi\rangle \langle \psi| = \hat{\rho}$$

since $\langle \psi | \psi \rangle = 1$.

Conversely, suppose that the density operator $\hat{\rho}$ is such that $\hat{\rho}^2 = \hat{\rho}$. We know that $\hat{\rho}$ can be written in the form

$$\hat{\rho} = \sum_{d=1}^{D} w_d \hat{P}_{|\psi_d\rangle}$$

for some collection of normalized states $\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_D\rangle\}$ and the real numbers $\{w_1, w_2, \ldots, w_D\}$.

Now, since the collection of states $\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_D\rangle\}$ is orthonormal, we have

$$\hat{P}_{|\psi_c\rangle} \hat{P}_{|\psi_d\rangle} = \delta_{cd} \hat{P}_{|\psi_d\rangle}$$

which implies that

$$\hat{\rho}^2 = \sum_{c=1}^{D} \sum_{d=1}^{D} w_c w_d \hat{P}_{|\psi_c\rangle} \hat{P}_{|\psi_d\rangle} = \sum_{c=1}^{D} \sum_{d=1}^{D} w_c w_d \delta_{cd} \hat{P}_{|\psi_d\rangle} = \sum_{d=1}^{D} w_d^2 \hat{P}_{|\psi_d\rangle}$$

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But we assumed that \( \hat{\rho}^2 = \hat{\rho} \) so that we must also have

\[
\hat{\rho}^2 = \sum_{d=1}^{D} w_d \hat{P}_{\psi_d}
\]

or

\[
\sum_{d=1}^{D} w_d^2 \hat{P}_{\psi_d} = \sum_{d=1}^{D} w_d \hat{P}_{\psi_d}
\]

Now, multiply both sides by \( \hat{P}_{\psi_c} \) and use \( \hat{P}_{\psi_c} \hat{P}_{\psi_d} = \delta_{cd} \hat{P}_{\psi_d} \)

\[
\sum_{d=1}^{D} w_d^2 \hat{P}_{\psi_c} \hat{P}_{\psi_d} = \sum_{d=1}^{D} w_d \hat{P}_{\psi_c} \hat{P}_{\psi_d}
\]

\[
\sum_{d=1}^{D} w_d^2 \delta_{cd} \hat{P}_{\psi_d} = \sum_{d=1}^{D} w_d \delta_{cd} \hat{P}_{\psi_d}
\]

\[
\langle w_c^2 - w_c \rangle \hat{P}_{\psi_c} = 0 \quad \text{for all} \ c = 1, 2, \ldots, D
\]

This implies that, for all \( c \), \( w_c^2 = w_c \). The only solution to this is \( w_c = 0 \) or 1. Since \( w_c > 0 \), we must have \( w_c = 1 \). However, we must also have

\[
\sum_{d=1}^{D} w_d^2 = 1 \rightarrow D = 1
\]

Therefore, \( \hat{\rho} = \hat{P}_{\psi} = |\psi\rangle \langle \psi| \) for some vector \( |\psi\rangle \) or \( \hat{\rho} \) represents a state vector.

### 6.19.2 Pure and Nonpure States

Consider an observable \( \sigma \) 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
  \[
  |\theta\rangle = \frac{1}{\sqrt{2}} |+\rangle + e^{i\theta} \frac{1}{\sqrt{2}} |--\rangle
  \]
  for arbitrary \( \theta \).

- (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?
Now, we have, in general, 
\[ \langle \sigma \rangle = Tr \hat{\rho} \hat{\sigma} \]
and 
\[ |\theta\rangle = \frac{1}{\sqrt{2}} |+\rangle + \frac{e^{i\theta}}{\sqrt{2}} |-\rangle \]
gives 
\[ \hat{\rho}_{\theta} = |\theta\rangle \langle \theta| = \frac{1}{2} |+\rangle \langle +| + \frac{1}{2} |-\rangle \langle -| + \frac{1}{2} e^{-i\theta} |+\rangle \langle -| + \frac{1}{2} e^{i\theta} |-\rangle \langle +| \]
Therefore, 
\[ \langle \sigma \rangle_{\theta} = Tr \hat{\rho}_{\theta} \hat{\sigma} = \langle +| \hat{\rho}_{\theta} \hat{\sigma} |+\rangle + \langle -| \hat{\rho}_{\theta} \hat{\sigma} |-\rangle \]
where 
\[ \hat{\sigma} = |+\rangle \langle +| - |-\rangle \langle -| \]
This gives 
\[ \langle \sigma \rangle_{\theta} = \langle +| \hat{\rho}_{\theta} |+\rangle - \langle -| \hat{\rho}_{\theta} |-\rangle = \frac{1}{2} - \frac{1}{2} = 0 \]
Similarly, for 
\[ \rho = \frac{1}{2} |+\rangle \langle +| + \frac{1}{2} |-\rangle \langle -| \]
we have 
\[ \langle \sigma \rangle = \langle +| \hat{\rho} |+\rangle - \langle -| \hat{\rho} |-\rangle = \frac{1}{2} - \frac{1}{2} = 0 \]
On the other hand, we also have that 
\[ \rho_{\theta} = \frac{1}{2} \begin{pmatrix} 1 & e^{i\theta} \\ e^{-i\theta} & 1 \end{pmatrix}, \quad \rho = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]
Now look at the operator 
\[ \sigma_{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]
We have 
\[ \rho_{\theta} \sigma_{x} = \frac{1}{2} \begin{pmatrix} e^{i\theta} & 1 \\ 1 & e^{-i\theta} \end{pmatrix}, \quad \rho \sigma_{x} = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]
Therefore, 
\[ \langle \sigma_{x} \rangle_{\theta} = Tr \hat{\rho}_{\theta} \hat{\sigma}_{x} = \frac{1}{2} (e^{i\theta} + e^{-i\theta}) = \cos \theta \rightarrow \text{represents a pure state} \]
\[ \langle \sigma_{x} \rangle = Tr \hat{\rho} \hat{\sigma}_{x} = 0 \rightarrow \text{represents a mixed state} \]
Therefore, for \( \hat{\rho} \), \( \langle \hat{B} \rangle = 0 \) for any \( \hat{B} \), for \( \hat{\rho}_{\theta} \), there exists an operator for which the result is certain (probability = 1), that is, \( \theta = 0 \).

This is so because \( |\theta = 0\rangle = |\sigma_{x} = +1\rangle \rightarrow \text{an eigenvector!} \)
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 \( \text{Prob}(M = 0|\rho) \) for the following state operators:

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

In problem 4.22.14 we showed that the eigenvalues of \( M \) are \( \lambda = 0, \pm \sqrt{2} \) and the corresponding eigenvectors of \( M \) are

\[ |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad |+\sqrt{2}\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}, \quad |\sqrt{2}\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \]

Now \( \hat{P}_0 = |0\rangle \langle 0| \) and we have, in general,

\[ \text{Prob}(M = 0|\rho) = \text{Tr}(\hat{P}_0\rho) = \langle M = 0| \hat{P}_0 \hat{\rho} | M = 0 \rangle + \langle M = \sqrt{2} | \hat{P}_0 \hat{\rho} | M = \sqrt{2} \rangle + \langle M = -\sqrt{2} | \hat{P}_0 \hat{\rho} | M = -\sqrt{2} \rangle \]

= \langle M = 0 | \hat{\rho} | M = 0 \rangle

(a) We have

\[ \rho = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \]

so that

\[ \text{Prob}(M = 0|\rho) = \langle M = 0 | \hat{\rho} | M = 0 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}^+ \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{3}{8} \]

(b) We have

\[ \rho = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \]

so that

\[ \text{Prob}(M = 0|\rho) = \langle M = 0 | \hat{\rho} | M = 0 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}^+ \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = 0 \]
(c) We have
\[
\rho = \begin{bmatrix}
\frac{1}{2} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & \frac{1}{2}
\end{bmatrix}
\]
so that
\[
Prob(M = 0|\rho) = \langle M = 0 | \hat{\rho} | M = 0 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{2} & 0 & 0 \\
0 & 0 & \frac{1}{2}
\end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2}
\]
Let us look at this in other ways to help our understanding of what is happening.

For the case
\[
\rho = \begin{bmatrix}
\frac{1}{2} & 0 & 0 \\
0 & \frac{1}{4} & 0 \\
0 & 0 & \frac{1}{4}
\end{bmatrix}
\]
Clearly, the eigenvalues of \( \hat{\rho} \) are \( 1/2, 1/4, 1/4 \). The corresponding eigenvectors are
\[
|1/2\rangle = |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1/4\rangle = |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |1/4\rangle = |-1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}
\]
Therefore the spectral decomposition of \( \hat{\rho} \) is
\[
\hat{\rho} = \frac{1}{2} |1\rangle \langle 1| + \frac{1}{4} |0\rangle \langle 0| + \frac{1}{4} |-1\rangle \langle -1| = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1
\end{bmatrix} + \frac{1}{4} \begin{bmatrix} 0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0
\end{bmatrix} + \frac{1}{4} \begin{bmatrix} 0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1
\end{bmatrix}
\]
Now, using the \( M \)-basis, we have
\[
|0\rangle = \frac{1}{\sqrt{2}} (|M = \sqrt{2}\rangle - |M = -\sqrt{2}\rangle)
\]
\[
|\pm 1\rangle = \frac{1}{\sqrt{2}} (|M = \sqrt{2}\rangle + |M = -\sqrt{2}\rangle) \pm \frac{1}{\sqrt{2}} |M = 0\rangle
\]
Therefore, we have
\[
\hat{\rho} = \frac{1}{2} |1\rangle \langle 1| + \frac{1}{4} |0\rangle \langle 0| + \frac{1}{4} |-1\rangle \langle -1| = \frac{1}{2} \begin{bmatrix}
\frac{1}{2} |M = \sqrt{2}\rangle \langle M = \sqrt{2}| + \frac{1}{2} |M = -\sqrt{2}\rangle \langle M = -\sqrt{2}| + \frac{1}{2} |M = 0\rangle \langle M = 0| \\
\frac{1}{2} |M = \sqrt{2}\rangle \langle M = -\sqrt{2}| + \frac{1}{2} |M = \sqrt{2}\rangle \langle M = 0| + \frac{1}{2} |M = -\sqrt{2}\rangle \langle M = 0| \\
\frac{1}{2} |M = 0\rangle \langle M = 0|
\end{bmatrix}
\]

and we have
\[
    \text{Prob}(M = 0|\rho) = \langle M = 0|\hat{\rho}|M = 0\rangle = \frac{11}{22} + \frac{11}{42} = \frac{3}{8}
\]
as before.

### 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.

\[
    \begin{align*}
    \rho_1 &= \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}, & \rho_2 &= \begin{bmatrix} \frac{5}{22} & \frac{12}{22} \\ \frac{12}{22} & \frac{5}{22} \end{bmatrix} \\
    \rho_3 &= \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix}, & \rho_4 &= \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \\
    \rho_5 &= \frac{1}{3} |u\rangle \langle u| + \frac{2}{3} |v\rangle \langle v| + \frac{\sqrt{2}}{3} |u\rangle \langle v| + \frac{\sqrt{2}}{3} |v\rangle \langle u|
    \end{align*}
\]

\[
    \begin{align*}
    \langle u|u\rangle = \langle v|v\rangle = 1 & \quad \text{and} \quad \langle u|v\rangle = 0 \\
    \rho_1 &= \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix} \rightarrow \rho_1^2 = \begin{bmatrix} \frac{5}{22} & \frac{12}{22} \\ \frac{12}{22} & \frac{5}{22} \end{bmatrix} \rightarrow \text{Tr}\rho_1^2 = \frac{7}{4} > 1 \quad \Rightarrow \quad \text{not acceptable} \\
    \rho_2 &= \begin{bmatrix} \frac{5}{22} & \frac{12}{22} \\ \frac{12}{22} & \frac{5}{22} \end{bmatrix} \rightarrow \rho_2^2 = \rho_2 \rightarrow \text{Tr}\rho_2^2 = \text{Tr}\rho_2 = 1 \quad \Rightarrow \quad \text{pure state} \\
    \rho_3 &= \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} = |\psi_3\rangle \langle \psi_3| \quad \Rightarrow \quad |\psi_3\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 3 \\ 4 \end{bmatrix} \\
    \rho_4 &= \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \rightarrow \rho_4^2 \neq \rho_4 \rightarrow \text{Tr}\rho_4^2 = \frac{5}{8} < 1 \quad \Rightarrow \quad \text{a mixed state}
    \end{align*}
\]

The eigenvalues of \(\rho_4\) are \(1/2, (1 \pm \sqrt{2})/4\) and the eigenvectors are
\[
    |1/2\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad \frac{1 + \sqrt{2}}{4} = \begin{bmatrix} 0.92 \\ 0 \\ 0.38 \end{bmatrix}, \quad \frac{1 - \sqrt{2}}{4} = \begin{bmatrix} -0.38 \\ 0 \\ 0.92 \end{bmatrix}
\]

Spectral decomposition implies that
\[
    \hat{\rho}_4 = \frac{1}{2} |1/2\rangle \langle 1/2| + \frac{1 + \sqrt{2}}{4} \left| 1 + \sqrt{2} \right\rangle \left\langle 1 + \sqrt{2} \right| + \frac{1 - \sqrt{2}}{4} \left| 1 - \sqrt{2} \right\rangle \left\langle 1 - \sqrt{2} \right|
\]

which corresponds to a mixed state.
\[
    \rho_5 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} \end{bmatrix} \rightarrow \rho_5^2 \neq \rho_5 \rightarrow \text{Tr}\rho_5^2 = \frac{1}{2} < 1 \quad \Rightarrow \quad \text{mixed state
\[ \rho_5 = \frac{1}{3} |u\rangle \langle u| + \frac{2}{3} |v\rangle \langle v| + \frac{\sqrt{2}}{3} |u\rangle \langle v| + \frac{\sqrt{2}}{3} |v\rangle \langle u| \quad , \quad \langle u \mid u \rangle = \langle v \mid v \rangle = 1 \text{ and } \langle u \mid v \rangle = 0 \]

\[ \rho_5^2 = \rho_5 \rightarrow \text{Tr} \rho_5^2 = \text{Tr} \rho_5 = 1 \rightarrow \text{pure state} \]

\[ \rho_5 = \frac{1}{\sqrt{3}} |u\rangle + \frac{\sqrt{2}}{3} |v\rangle \]

|ψ_5⟩ = 1 \frac{1}{\sqrt{3}} |u⟩ + \frac{\sqrt{2}}{3} |v⟩

### 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 \( 0 \leq r \leq 1 \).

We have \( \hat{\rho} = r \hat{\rho}_1 + (1-r) \hat{\rho}_2 \) where \( \hat{\rho}_1 \) and \( \hat{\rho}_2 \) are positive, semi-definite, which implies that

\[ \langle \psi \mid \hat{\rho}_1 \mid \psi \rangle \geq 0 \quad , \quad \langle \psi \mid \hat{\rho}_2 \mid \psi \rangle \geq 0 \]

and we also have \( 0 \leq (1-r) \leq 1 \). Therefore,

\[ \langle \psi \mid \hat{\rho} \mid \psi \rangle = r \langle \psi \mid \hat{\rho}_1 \mid \psi \rangle + (1-r) \langle \psi \mid \hat{\rho}_2 \mid \psi \rangle \]

This is the sum of two numbers both of which are greater than or equal to zero. Therefore,

\[ \langle \psi \mid \hat{\rho} \mid \psi \rangle \geq 0 \]

The trace is a linear operation, so

\[ \text{Tr} \hat{\rho} = r \text{Tr} \hat{\rho}_1 + (1-r) \text{Tr} \hat{\rho}_2 = r + (1-r) = 1 \]

Therefore, \( \hat{\rho} = r \hat{\rho}_1 + (1-r) \hat{\rho}_2 \) 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 |\( \tilde{\psi} \rangle = \hat{U} |\psi \rangle \) and |\( \tilde{\varphi} \rangle = \hat{U} |\varphi \rangle \), then \( \langle \tilde{\varphi} \mid \tilde{\psi} \rangle = \langle \varphi \mid \psi \rangle \) and \( \langle \tilde{\psi} \mid \tilde{\varphi} \rangle = \langle \psi \mid \varphi \rangle \).

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

We have

\[ \langle \tilde{\varphi} \mid \tilde{\psi} \rangle = \langle \varphi \mid U^+ U \mid \psi \rangle = \langle \varphi \mid \psi \rangle = \langle \varphi \mid I \mid \psi \rangle \]

\[ \Rightarrow U^+ U = I \]

\[ U^+ \tilde{\psi} = U^+ U \mid \psi \rangle = I \mid \psi \rangle = |\psi \rangle \]

\[ \Rightarrow \langle \varphi \mid \psi \rangle = \langle \tilde{\varphi} \mid U^+ U \mid \tilde{\psi} \rangle = \langle \tilde{\varphi} \mid \tilde{\psi} \rangle \]

\[ \Rightarrow UU^+ = I \]
(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.

Let

\[
U = \exp(iA), \quad A \text{ Hermitian}
\]

\[
U = \sum_{n=0}^{\infty} \frac{1}{n!} (iA)^n \Rightarrow U^+ = \sum_{n=0}^{\infty} \frac{1}{n!} (-iA)^n
\]

Thus,

\[
U^+ U = \exp(iA) \exp(-iA) = \exp(0) = I
\]

\( \Rightarrow \) \( U \) is unitary

where we have used \( e^A e^B = e^{A+B} \) when \( A \) and \( B \) commute.

(c) Let \( \hat{U}(t) = e^{-i\hat{H}t/\hbar} \) where \( t \) is time and \( \hat{H} \) is the Hamiltonian. Let \( |\psi(0)\rangle \) be the state at time \( t = 0 \). Show that \( |\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle \) 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.

Let \( U = e^{-iHt/\hbar} \), where \( H \) is the Hamiltonian. Given a state at \( t = 0 \), \( |\psi(0)\rangle \), let \( |\psi(t)\rangle = U(t) |\psi(0)\rangle \), which implies that

\[
\frac{\partial}{\partial t} |\psi(t)\rangle = \frac{\partial U(t)}{\partial t} |\psi(0)\rangle
\]

\[
\frac{\partial}{\partial t} U(t) = \frac{\partial e^{-iHt/\hbar}}{\partial t} = -\frac{iH}{\hbar} e^{-iHt/\hbar} = -\frac{iH}{\hbar} U(t)
\]

\[
\frac{\partial}{\partial t} |\psi(t)\rangle = -\frac{iH}{\hbar} U(t) |\psi(0)\rangle = -\frac{iH}{\hbar} |\psi(t)\rangle
\]

\[
i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle
\]

Thus, \( |\psi(t)\rangle = U(t) |\psi(0)\rangle \) is a solution of the Time Dependent Schrodinger equation.

The fact that \( |\psi\rangle \) evolves according to a unitary map is required by the probability interpretation of \( |\psi\rangle \). At \( t = 0 \), we choose \( ||\psi(0)\rangle||^2 = \langle\psi(0) | \psi(0)\rangle = 1 \), i.e., normalized to a total probability of all possible alternatives. At later times, this total probability must be conserved. This implies that

\[
||\psi(t)\rangle||^2 = \langle\psi(t) | \psi(t)\rangle = 1
\]

\[
\langle\psi(t) | \psi(t)\rangle = \langle\psi(0) | \psi(0)\rangle
\]

so that we have unitary time evolution.

(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 \( c_n \)?

Let the set \{\(|u_n\rangle\}\) (a complete orthonormal set) satisfy \( \hat{H} |u_n\rangle = E_n |u_n\rangle \).

This implies that

\[
\hat{I} = \sum_n |u_n\rangle \langle u_n |
\]

Thus,

\[
U(t) = U \hat{I} U = U \sum_n |u_n\rangle \langle u_n | = \sum_n e^{-iHt/\hbar} |u_n\rangle \langle u_n |
\]

and

\[
|\psi(t)\rangle = U(t) |\psi(0)\rangle = \left( \sum_n e^{-i\omega_n t} |u_n\rangle \langle u_n | \right) |\psi(0)\rangle = \sum_n e^{-i\omega_n t} |u_n\rangle \langle u_n | \psi(0)\rangle
\]

so that

\[
c_n = \langle u_n | \psi(0) \rangle
\]

### 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, \( \hat{J}_z \), 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 \( \rho \) 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.

Clearly \( \rho \) is hermitian and \( Tr \rho = 1 \). This is almost sufficient for \( \rho \) to be a valid density matrix. We can see this by noting that, given a hermitian matrix, we can make a transformation of basis to one in which \( \rho \) is diagonal. Such a transformation preserves the trace. In this diagonal basis, \( \rho \) is of the form

\[
\rho = a |1\rangle \langle 1| + b |2\rangle \langle 2| + c |3\rangle \langle 3|
\]

where \( a, b, c \) are real numbers (hermitian operators have real eigenvalues) such that \( a + b + c = 1 \) (trace = 1). This is clearly in the form of a density operator.

However, we must also have that \( \rho \) is positive, in the sense that \( a, b, c \) cannot be negative. Otherwise, we would interpret some probabilities as
negative. There are various ways to check this. For example, we can check that the expectation value of \( \rho \) with respect to any state is not negative. Thus let an arbitrary state be

\[
|\psi\rangle = \alpha |1\rangle + \beta |2\rangle + \gamma |3\rangle
\]

Then

\[
\langle \psi | \rho | \psi \rangle = (\alpha^* |1\rangle + \beta^* |2\rangle + \gamma^* |3\rangle) (a |1\rangle \langle 1| + b |2\rangle \langle 2| + c |3\rangle \langle 3|) (\alpha |1\rangle + \beta |2\rangle + \gamma |3\rangle)
\]

\[
= (\alpha^*, \beta^*, \gamma^*) \frac{1}{4} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}
\]

\[
= 2 |\alpha|^2 + |\beta|^2 + |\gamma|^2 + 2 \text{Re}(\alpha^* \beta) + 2 \text{Re}(\alpha^* \gamma)
\]

which can never be negative by virtue of the relation

\[
|x|^2 + |y|^2 + 2 \text{Re}(x^* y) = |x + y|^2 \geq 0
\]

Therefore, \( \rho \) is a valid density operator.

To determine whether \( \rho \) is a pure or mixed state, we consider

\[
\text{Tr}(\rho^2) = \frac{1}{16} \text{Tr} \begin{pmatrix} 6 & 3 & 3 \\ 3 & 2 & 1 \\ 3 & 1 & 2 \end{pmatrix} = \frac{5}{8}
\]

This is not equal to one, so \( \rho \) is a mixed state.

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

We are working in a diagonal basis for \( J_z \), therefore

\[
J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}
\]

The average value of \( J_z \) is then

\[
\langle J_z \rangle = \text{Tr}(\rho J_z) = \frac{1}{4} \text{Tr} \begin{pmatrix} 2 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix} = \frac{3}{4}
\]

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

We need

\[
\langle J_z^2 \rangle = \text{Tr}(\rho J_z^2) = \frac{1}{4} \text{Tr} \begin{pmatrix} 2 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \frac{3}{4}
\]

and then

\[
\Delta J_z = \sqrt{\langle J_z^2 \rangle - \langle J_z \rangle^2} = \sqrt{11/16} = 0.829
\]
6.19.8 Scale Transformation

Space is invariant under the scale transformation
\[ x \rightarrow x' = e^c x \]
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 \([\hat{D}, \hat{x}]\) and \([\hat{D}, \hat{p}_x]\) 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 6.19.11.

Under a scale transformation we have
\[ x \rightarrow x' = e^c x \]
which corresponds to the unitary transformation operator
\[ \hat{U} = e^{-ic\hat{D}} \]
where \( \hat{D} \) is the Hermitian dilation operator so that
\[ |x'\rangle = \hat{U} |x\rangle \]
The eigenvector/eigenvalue equation for these states is
\[ \hat{x} |x\rangle = x |x\rangle \]
which implies that
\[ \hat{x} U^{-1} |x'\rangle = x U^{-1} |x'\rangle = U^{-1} x |x'\rangle \rightarrow \hat{U} \hat{x} U^{-1} |x'\rangle = x |x'\rangle \]

Then
\[ \hat{U} \hat{x} U^{-1} |x'\rangle = x |x'\rangle = e^{-c} e^c x |x'\rangle = e^{-c} x' |x'\rangle = e^{-c} \hat{x} |x'\rangle \]
since
\[ \hat{x} |x'\rangle = x' |x'\rangle \]
This says that
\[ \hat{U} \hat{x} U^{-1} = e^{-c} \hat{x} \rightarrow e^c \hat{x} = U^{-1} \hat{x} \hat{U} = e^{ic\hat{D}} \hat{x} e^{-ic\hat{D}} \]
Now using the identity in Problem 6.19.11 we have
\[ e^{ic\hat{D}} \hat{x} e^{-ic\hat{D}} = \hat{x} + c \left[ i\hat{D}, \hat{x} \right] + \frac{1}{2} c^2 \left[ i\hat{D}, \left[ i\hat{D}, [i\hat{D}, \hat{x}] \right] \right] + \ldots \]
and also
\[ e^c \hat{x} = \hat{x} \left( 1 + c + \frac{1}{2} c^2 + \cdots \right) \]

These two powers series in \( c \) must be equal term-by-term so that we have
\[ \left[ i\hat{D}, \hat{x} \right] = \hat{x} \]

Now using the Jacobi identity we have
\[ \left[ \left[ \hat{D}, \hat{p}_x \right], \hat{x} \right] + \left[ \left[ \hat{p}_x, \hat{x} \right], \hat{D} \right] + \left[ \left[ \hat{x}, \hat{D} \right], \hat{p}_x \right] = 0 \]

Using \( [\hat{p}_x, \hat{x}] = -i\hbar \) and \( [\hat{x}, \hat{D}] = i\hbar \) we get
\[ \left[ \left[ \hat{D}, \hat{p}_x \right], \hat{x} \right] = \hbar \]

which says that
\[ \left[ \hat{D}, \hat{p}_x \right] = i\hbar \]

This says that
\[ \hat{D} = \frac{1}{\hbar} \left( \hat{x}\hat{p}_x + \hat{p}_x\hat{x} \right) \]

since
\[ \left[ i\hat{D}, \hat{x} \right] = \frac{i}{\hbar} \left[ \hat{x}\hat{p}_x + \hat{p}_x\hat{x}, \hat{x} \right] = \frac{i}{\hbar} \left( [\hat{x}\hat{p}_x, \hat{x}] + [\hat{p}_x\hat{x}, \hat{x}] \right) = \frac{i}{\hbar} \left( -i\hbar \hat{x} - i\hbar \hat{x} \right) = \hat{x} \]
\[ -i\hat{D}, \hat{p}_x \right] = \frac{-i}{\hbar} \left[ \hat{x}\hat{p}_x + \hat{p}_x\hat{x}, \hat{p}_x \right] = \frac{-i}{\hbar} \left( [\hat{x}\hat{p}_x, \hat{p}_x] + [\hat{p}_x\hat{x}, \hat{p}_x] \right) = \frac{-i}{\hbar} \left( i\hbar \hat{p}_x + i\hbar \hat{p}_x \right) = \hat{p}_x \]

and \( \hat{D} \) must be hermitian.

6.19.9 Operator Properties

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

We have
\[ U = e^{i\hat{H}} \]

Then
\[ \hat{U}^+ = e^{-i\hat{H}^+} = e^{-i\hat{H}} \]
\[ \hat{U}^+ \hat{U} = e^{-i\hat{H}} e^{i\hat{H}} = \hat{1} \]

so that \( \hat{U} \) is unitary.

(b) Show that \( \det U = e^{iTr\hat{H}} \).

There exists a unitary matrix \( U \) that diagonalizes \( H \), i.e.,
\[ U^+ H U = D \]

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Then
\[ U^+ H^2 U = U^+ HUU^+ H U = D^2 \]
and
\[ U^+ H^n U = U^+ HU \ldots U^+ H U = D^n \]

We then have
\[ U^+ e^{iH} U = \sum_{n=0}^{\infty} U^+ (iH)^n U = \sum_{n=0}^{\infty} U^+ (iD)^n U = U^+ e^{iD} U \]

Now since \( D \) is diagonal and since the product of diagonal matrices is also diagonal we get
\[
(e^{iD})_{ii} = \sum_{n=0}^{\infty} \frac{(iD)^n}{n!} = e^{iD_{ii}} \rightarrow e^{iD} = \begin{bmatrix}
e^{i\lambda_1} & 0 & 0 & 0 & \ldots & 0 \\
0 & e^{i\lambda_2} & 0 & 0 & \ldots & 0 \\
0 & 0 & e^{i\lambda_3} & 0 & \ldots & 0 \\
0 & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & 0 & \ldots & \ldots & e^{i\lambda_n} \end{bmatrix}
\]

and
\[
det(U) = det(e^{iH}) = det(e^{iH}UU^+) = det(U^+ e^{iH} U) = det(e^{iD})
= e^{i\lambda_1} e^{i\lambda_2} e^{i\lambda_3} \ldots e^{i\lambda_n} = e^{i(\lambda_1+\lambda_2+\lambda_3+\ldots+\lambda_n)} = e^{iTrD}
\]

Now
\[ Tr(U^+ H U) = Tr(HUU^+) = TrH = TrD = \sum_{i} \lambda_i \]
so that
\[ det(U) = e^{iTrD} = e^{iTrH} \]

### 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:
\[ \hat{U} \hat{V} \hat{U}^{-1} = \hat{V} - \vec{v} \hat{I}, \quad \hat{U} \hat{Q} \hat{U}^{-1} = \hat{Q} \]

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
\[ \hat{U} \hat{V} \hat{U}^{-1} = \hat{V} - \vec{v} \hat{I}, \quad \hat{U} \hat{Q} \hat{U}^{-1} = \hat{Q} - \vec{v} \hat{I} \]
Verify that \( \hat{G}_t \) satisfies the same commutation relation with \( \hat{P}, \hat{J} \) and \( \hat{H} \) as does \( \hat{G} \).

The restricted Galilean transformation is given by the unitary operator \( \hat{U}(\vec{v}) = e^{i\vec{v} \cdot \hat{G}} \) such that
\[
\hat{U} \hat{V} \hat{U}^{-1} = \hat{V} - \vec{v} \hat{I} , \quad \hat{U} \hat{Q} \hat{U}^{-1} = \hat{Q}
\]
This restricted transformation is *instantaneous* and thus causes no change in the position!

The full Galilean transformation is given by \( \hat{U}(\vec{v},t) = e^{i\vec{v} \cdot \hat{G}_t} \) such that
\[
\hat{U} \hat{V} \hat{U}^{-1} = \hat{V} - \vec{v} \hat{I} , \quad \hat{U} \hat{Q} \hat{U}^{-1} = \hat{Q} - \vec{v}t \hat{I}
\]

**Method 1:**
\[
e^{i\vec{v} \cdot \hat{G}_t} \hat{Q} e^{-i\vec{v} \cdot \hat{G}_t} = \hat{Q} + i \left[ \vec{v} \cdot \hat{G}_t, \hat{Q} \right] + ....
\]
which implies that
\[
\hat{G}_t = -\frac{\hat{P}}{\hbar} t + \frac{1}{\hbar} \hat{Q}
\]
that is,
\[
i \left[ \vec{v} \cdot \hat{G}_t, \hat{Q} \right] = iv_x \left[ \hat{G}_{tx}, \hat{x} \right] + iv_y \left[ \hat{G}_{ty}, \hat{y} \right] + iv_z \left[ \hat{G}_{tz}, \hat{z} \right]
\]
\[
= iv_x \left( -\frac{t}{\hbar} \right) \left[ \hat{P}_x, \hat{x} \right] + iv_y \left[ \hat{P}_y, \hat{y} \right] + iv_z \left[ \hat{P}_z, \hat{z} \right] = -\vec{v} t \hat{I}
\]
as expected.

**Method 2:** The desired transformation \( \hat{U}(\vec{v},t) = e^{i\vec{v} \cdot \hat{G}_t} \) is a combination of an instantaneous Galilean transformation, which affects the velocity operator, but not the position operator, and a space displacement through the distance \( \vec{v} t \).
This suggests that we try
\[
\hat{G}_t = (\text{instantaneous boost}) + (\text{space translation})
\]
We let \( \hbar = 1 \) for convenience. We have
\[
e^{i\vec{v} \cdot \hat{G}_t} \hat{Q}_\alpha e^{-i\vec{v} \cdot \hat{G}_t} = \hat{Q}_\alpha + \left[ i\vec{v} \cdot \hat{G}_t, \hat{Q}_\alpha \right] + ( \text{higher order terms} )
\]
The commutator has the value
\[
\left[ i\vec{v} \cdot \hat{G}_t, \hat{Q}_\alpha \right] = -i \left[ i\vec{v} \cdot \hat{P}_t, \hat{Q}_\alpha \right] = -v_\alpha t \hat{I}
\]
Since this is a multiple of the identity operator, all the higher order terms vanish above and we get
\[ e^{i\vec{v} \cdot \hat{G}_t} \hat{Q}_\alpha e^{-i\vec{v} \cdot \hat{G}_t} = \hat{Q}_\alpha - v_\alpha t \hat{I} \]

Similarly,
\[ e^{i\vec{v} \cdot \hat{G}_t} \hat{P}_\alpha e^{-i\vec{v} \cdot \hat{G}_t} = \hat{P}_\alpha + \left[ i\vec{v} \cdot \hat{G}_t, \hat{P}_\alpha \right] + \text{(higher order terms)} \]
\[ \left[ i\vec{v} \cdot \hat{G}_t, \hat{P}_\alpha \right] = -i \left[ iM\vec{v} \cdot \hat{Q}, \hat{P}_\alpha \right] = -Mv_\alpha \hat{I} \]

Again all higher order terms are zero and we have
\[ e^{i\vec{v} \cdot \hat{G}_t} \hat{P}_\alpha e^{-i\vec{v} \cdot \hat{G}_t} = \hat{P}_\alpha - Mv_\alpha t \hat{I} \]

Dividing the equation by \( M \) gives the correct transformation equation for the velocity operator \( \hat{V}_\alpha = \hat{P}_\alpha / M \). So the assumption
\[ \hat{G}_t = M\hat{Q} - t\hat{P} \]

is correct.

**Commutators**: Consider \( \hat{G}_{t_1} \) with \( \hat{H} \). We have
\[ e^{ix\hat{H}} e^{i\vec{v} \cdot \hat{G}_{t_1}} e^{-i\vec{v} \cdot \hat{G}_{t_1}} = \hat{I} + x^2 \left[ \hat{G}_{t_1}, \hat{H} \right] \]

This is unchanged from result in text with \( \hat{G}_1 \) and so this commutator does not change and similarly for all others.

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

There is a clever way (see Problem 6.19.12 below if you are having difficulty) to do this problem using ODEs and not just brute-force multiplying everything out. Straightforward expansion/regrouping
\[ \hat{f}(x) = e^{x\hat{A}} \hat{B} e^{-x\hat{A}} = \left( \sum_n \frac{(x\hat{A})^n}{n!} \right) \hat{B} \left( \sum_n \frac{(-x\hat{A})^n}{n!} \right) \]
\[ = \left( 1 + x\hat{A} + \frac{1}{2} x^2 \hat{A}^2 + \ldots \right) \hat{B} \left( 1 - x\hat{A} + \frac{1}{2} x^2 \hat{A}^2 - \ldots \right) \]
\[ = \hat{B} + x \left[ \hat{A}, \hat{B} \right] + x^2 \left( -\hat{A}\hat{B}\hat{A} + \frac{1}{2} (\hat{A}^2\hat{B} - \hat{B}\hat{A}^2) \right) + \ldots \]
\[ = \hat{B} + x \left[ \hat{A}, \hat{B} \right] + \frac{1}{2} x^2 \left( \hat{A}(\hat{A}\hat{B} - \hat{B}\hat{A}) - (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{A} \right) + \ldots \]
\[ = \hat{B} + x \left[ \hat{A}, \hat{B} \right] + \frac{1}{2} x^2 \left[ \hat{A}, \left[ \hat{A}, \hat{B} \right] \right] + \ldots \]
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

\[
e^A Be^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} \left[ A, [A, [A, ..., [A, B]...]] \right]_n
\]

\[
= B + [A, B] + \frac{1}{2!} [A, [A, B]] + \frac{1}{3!} [A, [A, [A, B]]] + ....
\]

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

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

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

(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 expression, show that \( B_n = [A, B_{n-1}] / n \).

First, note that

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

Now, integrating, we have

\[
B(1) = B + \int_0^1 dt \frac{d}{dt} B(t) dt
\]

\[
B(1) = B + \int_0^1 [A, B(t)] dt
\]

\[
\sum_{n=0}^{\infty} B_n = B_0 + \sum_{n=0}^{\infty} [A, B_n] \int_0^1 t^n dt
\]

\[
\sum_{n=0}^{\infty} B_n = B_0 + \sum_{n=0}^{\infty} [A, B_n] \frac{1}{n + 1}
\]

\[
\sum_{n=0}^{\infty} B_n = \sum_{n=0}^{\infty} [A, B_n] \frac{1}{n + 1}
\]

\[
\sum_{n=1}^{\infty} B_n = \sum_{n=1}^{\infty} [A, B_{n-1}] \frac{1}{n}
\]

\[
\rightarrow B_n = \frac{1}{n} [A, B_{n-1}]
\]
(c) Show by induction that
\[ B_n = \frac{1}{n!} \underbrace{[A, [A, ... [A, B] ... ]]}_{n} \]

We have
\[ B_n = \frac{1}{n} [A, B_{n-1}] = \frac{1}{n} \left[ A, \frac{1}{n-1} [A, B_{n-2}] \right] \]
\[ = \frac{1}{n(n-1)} [A, [A, B_{n-2}]] = \ldots = \frac{1}{n(n-1) \ldots (n-n+1)} [A, \ldots [A, B_{n-n}]] \]
\[ = \frac{1}{n!} [A, [A, \ldots [A, B] \ldots ]] \quad \text{(with } n \text{ nested commutators)} \]

(d) Use \( B(1) = e^A B e^{-A} \) and prove the identity.
\[
e^A B e^{-A} = B(1) = \sum_{n=0}^{\infty} B_n
\]
\[
= \sum_{n=0}^{\infty} \frac{1}{n!} [A, [A, \ldots [A, B] \ldots ]]\]

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

We have \( A = ipa/\hbar \), so that
\[
e^{ipa/\hbar} xe^{-ipa/\hbar} = \sum_{n=0}^{\infty} \frac{1}{n!} [A, [A, \ldots [A, x] \ldots ]]
\]
\[
= \sum_{n=0}^{\infty} \frac{a^n}{n!} \left( \frac{i}{\hbar} \right)^n [p, [p, \ldots [p, x] \ldots ]]
\]

Only the first and second terms survive so that
\[
e^{ipa/\hbar} xe^{-ipa/\hbar} = x + a \left( \frac{i}{\hbar} \right) (-i\hbar) = x + a
\]

**Alternative Method:** Let \( \hat{f}(x) = e^{x\hat{A}} \hat{B} e^{-x\hat{A}} \) where \( x \) is a parameter. In general, we can write
\[
\hat{f}(x) = \hat{f}(0) + x \frac{d\hat{f}(x)}{dx} \bigg|_{x=0} + \frac{1}{2} x^2 \frac{d^2\hat{f}(x)}{dx^2} \bigg|_{x=0} + \ldots
\]

In this case, we can write
\[
\frac{d\hat{f}(x)}{dx} = \hat{A} e^{x\hat{A}} \hat{B} e^{-x\hat{A}} - e^{x\hat{A}} \hat{B} e^{-x\hat{A}} \hat{A} = [\hat{A}, \hat{f}(x)]
\]
This implies that
\[ \frac{d^2 \hat{f}(x)}{dx^2} = \frac{d}{dx} \left[ \frac{df}{dx} \right] = \frac{d}{dx} \left[ \hat{A}, \hat{f}(x) \right] = \left[ \hat{A}, \left[ \hat{A}, \hat{f}(x) \right] \right] \]
and so on. Since \( \hat{f}(0) = \hat{B} \) we get
\[ \hat{f}(x) = e^{x \hat{A}} \hat{B} e^{-x \hat{A}} = \hat{B} + \left[ \hat{A}, \hat{B} \right] x + \left[ \hat{A}, [\hat{A}, \hat{B}] \right] \frac{x^2}{2} + \left[ \hat{A}, [\hat{A}, [\hat{A}, \hat{B}]] \right] \frac{x^3}{6} + \ldots \]
We note that this is the solution of the first-order operator differential equation
\[ \frac{df(x)}{dx} = \left[ \hat{A}, f(x) \right] \]
with boundary condition \( \hat{f}(0) = \hat{B} \).

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
\[ [\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0 \]
A clever solution uses Problem 6.11 or 6.12 result and ODEs.

We define \( \hat{f}(x) = e^{x \hat{A}} e^{x \hat{B}} \). We then have
\[ \frac{d\hat{f}(x)}{dx} = \hat{A} e^{x \hat{A}} e^{x \hat{B}} + e^{x \hat{A}} \hat{B} e^{x \hat{A}} e^{x \hat{B}} = \hat{A} e^{x \hat{A}} e^{x \hat{B}} + e^{x \hat{A}} \hat{B} e^{-x \hat{A}} e^{x \hat{A}} e^{x \hat{B}} \]
\[ = \left( \hat{A} + e^{x \hat{A}} \hat{B} e^{-x \hat{A}} \right) e^{x \hat{A}} e^{x \hat{B}} = \left( \hat{A} + e^{x \hat{A}} \hat{B} e^{-x \hat{A}} \right) \hat{f}(x) \]
Since \( [\hat{A}, [\hat{A}, \hat{B}]] = 0 \), problems 6.19.11 and 6.19.12 say
\[ e^{x \hat{A}} \hat{B} e^{-x \hat{A}} = \hat{B} + \left[ \hat{A}, \hat{B} \right] x \]
so that we have
\[ \frac{d\hat{f}(x)}{dx} = \left( \hat{A} + e^{x \hat{A}} \hat{B} e^{-x \hat{A}} \right) \hat{f}(x) = \left( \hat{A} + \hat{B} + [\hat{A}, \hat{B}] x \right) \hat{f}(x) \]
This equation has the solution
\[ \hat{f}(x) = e^{x \hat{A}} e^{x \hat{B}} = e^{(\hat{A} + \hat{B})x + \frac{1}{2} x^2 [\hat{A}, \hat{B}]} \]
If we choose $x = 1$ we have
\[ e^{\hat{A}}e^{\hat{B}} = e^{(\hat{A} + \hat{B}) + \frac{1}{2}[\hat{A}, \hat{B}]} = e^{\hat{A} + \hat{B}}e^{\frac{1}{2}[\hat{A}, \hat{B}]} \]
where the last step follows because
\[ [\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0 \]
(behavior like ordinary numbers in algebra). Therefore, we finally get
\[ e^{\hat{A} + \hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A}, \hat{B}]} \]

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.

We have
\[ \frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} \left[ \hat{H}(t), \hat{\rho}(t) \right] \]
For a pure state we have $Tr\hat{\rho}^2 = 1$ (not < 1) and $\hat{\rho} = |\psi\rangle \langle \psi|$ (a single projection operator and NOT a sum). Therefore,
\[ \frac{dTr\hat{\rho}^2}{dt} = Tr\frac{d\hat{\rho}^2}{dt} = 2Tr\hat{\rho}\frac{d\hat{\rho}}{dt} = -\frac{2i}{\hbar}Tr\left( \hat{\rho} \left[ \hat{H}, \hat{\rho} \right] \right) \]
Using $TrAB = TrBA$, we have
\[ \frac{dTr\hat{\rho}^2}{dt} = -\frac{2i}{\hbar}Tr\left( \hat{\rho} \left[ \hat{H}, \hat{\rho} \right] \right) = \frac{2i}{\hbar}Tr\left( \hat{\rho}\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\hat{\rho} \right) = 0 \]
so that
\[ Tr\hat{\rho}^2(t) = Tr\hat{\rho}^2(0) = 1 = \text{constant} \]
this says that a pure state cannot change into a nonpure or mixed state.

Alternatively,
\[ Tr\hat{\rho}^2(t) = Tr(\hat{\rho}(t)\hat{\rho}(t)) = Tr \left( \hat{U}\hat{\rho}(t_0)\hat{U}^{-1}\hat{U}\hat{\rho}(t_0)\hat{U}^{-1} \right) \]
\[ = Tr \left( \hat{U}\hat{\rho}(t_0)\hat{I}\hat{\rho}(t_0)\hat{U}^{-1} \right) = Tr \left( \hat{U}\hat{\rho}(t_0)\hat{\rho}(t_0)\hat{U}^{-1} \right) \]
\[ = Tr \left( \hat{\rho}(t_0)\hat{I}\hat{\rho}(t_0)\hat{U}^{-1}\hat{U} \right) = Tr(\hat{\rho}(t_0)\hat{I}\hat{\rho}(t_0)) = Tr\hat{\rho}^2(t_0) \]
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

\[
\hat{q}g(x) = xg(x) \quad \hat{p}g(x) = -i \frac{dg(x)}{dx} = -ig'(x)
\]

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 \( \tilde{G} \)

We shall equip the space \( \tilde{G} \) with the scalar product

\[
S(f, g) = \int_{-\infty}^{\infty} dx f^*(x)g(x)
\]

for any \( f \) and \( g \) in \( \tilde{G} \). Clearly,

\[
S(f, \hat{q}g) = \int_{-\infty}^{\infty} dx x f^*(x)g(x)
\]

On the other hand,

\[
S(f, \hat{q}^+ g) = S(\hat{q}f, g) = \int_{-\infty}^{\infty} dx x f^*(x)g(x)
\]

since \( x \) is real. Hence \( S(f, \hat{q}g) = S(f, \hat{q}^+ g) \) for all \( f \) and \( g \) in \( \tilde{G} \), and thus

\( \hat{q} = \hat{q}^+ \)

For the operator \( \hat{p} \)

\[
S(f, \hat{p}g) = -i \int_{-\infty}^{\infty} dx f^*(x)g'(x)
\]

and

\[
S(f, \hat{p}^+ g) = S(\hat{p}f, g) = \int_{-\infty}^{\infty} dx [-if^*(x)]'g(x) = i \int_{-\infty}^{\infty} dx f^*(x)g(x)
\]

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If we perform an integration by parts, we have
\[
S(f, \hat{p}^+ g) = i \int_{-\infty}^{\infty} dx f^*(x)g(x) = i [f(\infty)g(\infty) - f(-\infty)g(-\infty)] - i \int_{-\infty}^{\infty} dx f^*(x)g'(x)
\]
Now the integrated term vanishes, since by definition of the scalar product, the functions \( f \) and \( g \) must vanish on the boundary. Therefore,
\[
\hat{p} = \hat{p}^+
\]
(2) \( \hat{M} \) is a constant multiple of the identity operator

Since \( [\hat{M}, \hat{q}] = 0 \), it follows that \( [\hat{M}, \hat{q}^n] = 0 \), \( n = 1, 2, 3, \ldots \) and hence that
\[
[\hat{M}, e^{it\hat{q}}] = 0
\]
Thus, any function of the operator \( \hat{q} \) that has a Fourier transform,
\[
f(\hat{q}) = \int_{-\infty}^{\infty} dt \hat{f}(t)e^{it\hat{q}}
\]
also commutes with \( \hat{M} \). For such a function,
\[
\hat{M}f(\hat{q})g(x) = f(\hat{q})\hat{M}g(x)
\]
Since \( \hat{q}g(x) = xg(x) \), \( \hat{q}^n g(x) = x^n g(x) \) and \( e^{it\hat{q}} g(x) = e^{itx} g(x) \) so that
any function with a Fourier transform satisfies \( f(\hat{q})g(x) = f(x)g(x) \), then
\[
\hat{M}f(x)g(x) = f(\hat{q})\hat{M}g(x)
\]
If we now choose \( g(x) = 1 \), we have
\[
\hat{M}f(x) = f(\hat{q})m(x) = f(x)m(x)
\]
where \( \hat{M}g(x) = m(x) \) when \( g(x) = 1 \).

Certainly, the unit function belongs to \( \tilde{G} \) and we are sure that the function \( m(x) \) lies in the space \( \tilde{G} \) (this is the reason why we extended the space of test functions from \( G \) to \( \tilde{G} \) - in \( G \) the above statements are not true!). We can now replace \( f(x) \) by \( g(x) \) or \( g'(x) \) (they also have Fourier transforms) so that we have
\[
\hat{M}g(x) = g(x)m(x) \quad , \quad \hat{M}g'(x) = g'(x)m(x)
\]
Now consider the fact that \( \hat{M} \) commutes with \( \hat{p} \). Thus implies that
\[
\hat{p}\hat{M}g(x) = \hat{M}\hat{p}g(x) = -i\hat{M}g'(x) = -ig'(x)m(x)
\]
\[
\hat{p}\hat{M}g(x) = \hat{p}g(x)m(x) = -i\frac{d}{dx}(g(x)m(x))
\]
\[
-\frac{d}{dx}(g(x)m(x)) = -ig'(x)m(x)
\]
\[
\frac{d}{dx}(g(x)m(x)) = g'(x)m(x)
\]
This last result implies that \( m'(x) = 0 \) or \( m(x) = \kappa \), a constant.

We then have

\[
\hat{M}g(x) = \kappa g(x)
\]

or, in other words, \( \hat{M} = \kappa \hat{I} \) where \( \hat{I} \) is the identity operator on \( G \).

### 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 \( \rho \) 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.

The density matrix \( \rho \) is hermitian, hence diagonal in some basis. Work in such a basis. In this basis, \( \rho \) has the form

\[
\rho = \begin{pmatrix}
\theta & 0 \\
0 & 1 - \theta
\end{pmatrix}
\]

where \( 0 \leq \theta \leq 1 \) is the probability that the system is in state 1. We have a pure state if and only if either \( \theta = 1 \) or \( \theta = 0 \). The entropy is

\[
s = -\theta \ln \theta - (1 - \theta) \ln (1 - \theta)
\]

(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 \( \rho \).

Figure 6.1: The entropy as a function of \( \theta \)
The entropy for a pure state, with $\theta = 1$ or $\theta = 0$, is zero. The entropy increases as the state becomes less pure, reaching a maximum when the probability of being in either state is $1/2$, reflecting minimal knowledge about the state.

(c) Consider a system with ensemble $\rho$ a mixture of two ensembles $\rho_1$ and $\rho_2$:

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

As an example, suppose

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

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.

The entropy of ensemble 1 is:

$$s(\rho_1) = -Tr\rho_1 \ln \rho_1 = -\frac{1}{2} \ln \frac{1}{2} - \frac{1}{2} \ln \frac{1}{2} = \ln 2 = 0.6931$$

It may be noticed that $\rho_2^2 = \rho_2$, hence ensemble 2 is a pure state, with entropy $s(\rho_2) = 0$. Next, we need the entropy of the combined ensemble:

$$\rho = \theta \rho_1 + (1 - \theta) \rho_2 = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 - \theta & 1 - \theta \end{pmatrix}$$

To compute the entropy, it is convenient to determine the eigenvalues, they are $1 - \theta/2$ and $\theta/2$. Note that they are in the range from zero to one, as they must be. The entropy is

$$s(\rho) = -\left(1 - \frac{\theta}{2}\right) \ln \left(1 - \frac{\theta}{2}\right) - \left(-\frac{\theta}{2}\right) \ln \left(-\frac{\theta}{2}\right)$$

We must compare $s(\rho)$ with

$$\theta s(\rho_1) + (1 - \theta) s(\rho_2) = \theta \ln 2$$

It is readily checked that equality holds for $\theta = 1$ or $\theta = 0$. For the case $0 < \theta < 1$, take the difference of the two expressions:

$$s(\rho) - [\theta s(\rho_1) + (1 - \theta) s(\rho_2)] = -\left(1 - \frac{\theta}{2}\right) \ln \left(1 - \frac{\theta}{2}\right) - \left(-\frac{\theta}{2}\right) \ln \left(-\frac{\theta}{2}\right) - \theta \ln 2$$

$$= \ln \left[\left(1 - \frac{\theta}{2}\right)^{1 - \theta/2} \left(\frac{\theta}{2}\right)^{\theta/2} 2^\theta\right]$$

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This must be larger than zero if the mixing theorem is correct. This is equivalent to asking whether

\[
\left(1 - \frac{\theta}{2}\right)^{1 - \theta/2} \left(\frac{\theta}{2}\right)^{\theta/2} 2^\theta
\]

is less than 1. This expression may be rewritten as

\[
\left(1 - \frac{\theta}{2}\right)^{1 - \theta/2} (2\theta)^{\theta/2}
\]

It must be less than 1. To check, let us find its maximum value, by setting its derivative with respect to \(\theta\) equal to 0:

\[
0 = \frac{d}{d\theta} \left(1 - \frac{\theta}{2}\right)^{1 - \theta/2} (2\theta)^{\theta/2}
= \frac{d}{d\theta} \exp \left[ \left(1 - \frac{\theta}{2}\right) \ln \left(1 - \frac{\theta}{2}\right) + \left(\frac{\theta}{2}\right) \ln (2\theta) \right]
= -\frac{1}{2} \ln (1 - \theta/2) + \frac{1}{2} \ln (2\theta) - \frac{1}{2} + \frac{2}{4}
= \ln (2\theta) - \ln (1 - \theta/2)
\]

Thus, the maximum occurs at \(\theta = 2/5\). At this value of \(\theta\), \(s(\rho) = 0.500\), and \(\theta s(\rho_1) + (1 - \theta)s(\rho_2) = (2/5) \ln 2 = 0.277\). The theorem holds.

### 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 \(\zeta\) of the reduced density operator \(\tilde{\rho}_A = \text{Tr}_B[|\Psi_{AB}\rangle \langle \Psi_{AB}|]\) given by

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

is a good measure of the entanglement of states in \(\mathcal{H}_{AB}\). For pure states of the above form, find extrema of \(\zeta\) with respect to \(\theta\) \((0 \leq \theta \leq \pi/2)\). Do entangled states have large \(\zeta\) or small \(\zeta\)? We first form the density operator corresponding to \(|\Psi_{AB}\rangle\),

\[
\rho = |\Psi_{AB}\rangle \langle \Psi_{AB}|
= \cos^2 \theta |00\rangle \langle 00| + \cos \theta \sin \theta |00\rangle \langle 11| + \cos \theta \sin \theta |11\rangle \langle 00| + \sin^2 \theta |11\rangle \langle 11|
\]

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Here $|\Psi_{00}\rangle$ stands for $|0_A\rangle \otimes |0_B\rangle$, and so forth. Now we take the partial trace over $A$ to find the reduced density operator,

$$\tilde{\rho}_A = Tr_B \rho = \langle 0_B | \rho | 0_B \rangle + \langle 1_B | \rho | 1_B \rangle$$

$$= \cos^2 \theta |0_A\rangle \langle 0_A| + \sin^2 \theta |1_A\rangle \langle 1_A|$$

and then

$$\tilde{\rho}^2_A = \cos^4 \theta |0_A\rangle \langle 0_A| + \sin^4 \theta |1_A\rangle \langle 1_A|$$

so that

$$\zeta = Tr[\tilde{\rho}^2_A] = \cos^4 \theta + \sin^4 \theta$$

The extrema correspond to

$$\zeta' = \frac{d\zeta}{d\theta} = -4 \cos^3 \theta \sin \theta + 4 \sin^3 \theta \cos \theta = 0$$

which gives

$$\cos^3 \theta \sin \theta = \sin^3 \theta \cos \theta \rightarrow \cos^2 \theta = \sin^2 \theta$$

For $0 \leq \theta \leq \pi/2$, this equation is satisfied for $\theta = \pi/4$, $\cos^2 \theta = \sin^2 \theta = 1/2$ and also $\zeta = 1/2$. At $\theta = \pi/4$,

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

which we recognize as a highly entangled state. Since for $\theta = 0$ we have

$$|\Psi_{AB}\rangle \rightarrow |0_A\rangle \otimes |0_B\rangle$$

which is unentangled and $\zeta \rightarrow 1$, we see clearly that entangled states are associated with smaller purity for the reduced density operator.

### 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),

$$U_{AB} = P^A_0 \otimes I^B + P^A_1 \otimes \sigma^B_x$$

where $P^A_0 = |0_A\rangle \langle 0_A|$, $P^A_1 = |1_A\rangle \langle 1_A|$ and $\sigma^B_x = |0_B\rangle \langle 1_B| + |1_B\rangle \langle 0_B|$. 

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?
We start by writing out
\[
U_{AB} = P_0^A \otimes I^B + P_1^A \otimes \sigma_x^B
= |0_A\rangle \langle 0_A| \otimes |0_B\rangle \langle 0_B| + |0_A\rangle \langle 0_A| \otimes |1_B\rangle \langle 1_B|
+ |1_A\rangle \langle 1_A| \otimes |0_B\rangle \langle 1_B| + |1_A\rangle \langle 1_A| \otimes |1_B\rangle \langle 0_B|
= |0_A\rangle \otimes |0_B\rangle \langle 0_A| \langle 0_B| + |0_A\rangle \otimes |1_B\rangle \langle 0_A| \langle 1_B|
+ |1_A\rangle \otimes |0_B\rangle \langle 1_A| \langle 1_B| + |1_A\rangle \otimes |1_B\rangle \langle 1_A| \langle 0_B|
\]

Hence, in the basis order given,
\[
U_{AB} \rightarrow \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
\]

We see immediately that
\[
\begin{pmatrix}
1 \\
0 \\
0 \\
0
\end{pmatrix} \leftrightarrow |0_A\rangle \otimes |0_B\rangle, \quad \begin{pmatrix}
0 \\
1 \\
0 \\
0
\end{pmatrix} \leftrightarrow |0_A\rangle \otimes |1_B\rangle
\]

are unentangled eigenstates of \(U_{AB}\). Then from prior experience we can also guess that
\[
\frac{1}{\sqrt{2}} \begin{pmatrix}
0 \\
0 \\
1 \\
1
\end{pmatrix} \leftrightarrow \frac{1}{\sqrt{2}} (|1_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle) = |1_A\rangle \otimes (|0_B\rangle + |1_B\rangle)
\]
\[
\frac{1}{\sqrt{2}} \begin{pmatrix}
0 \\
0 \\
1 \\
-1
\end{pmatrix} \leftrightarrow \frac{1}{\sqrt{2}} (|1_A\rangle \otimes |0_B\rangle - |1_A\rangle \otimes |1_B\rangle) = |1_A\rangle \otimes (|0_B\rangle - |1_B\rangle)
\]

Neither of these are entangled either.

6.19.19 Creating Entanglement via Unitary Evolution

Working with the same system as in Problems 6.19.17 and 6.19.18, find a factorizable input state
\[
|\Psi_{in}^{AB}\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle
\]
such that the output state
\[
|\Psi_{out}^{AB}\rangle = U_{AB} |\Psi_{in}^{AB}\rangle
\]
is maximally entangled. That is, find any factorizable \(|\Psi_{in}^{AB}\rangle\) such that
\[
\text{Tr} [\tilde{\rho}_A^2] = \frac{1}{2},
\]
where
\[
\tilde{\rho}_A = \text{Tr}_B [ |\Psi_{out}^{AB}\rangle \langle \Psi_{out}^{AB}|]
\]

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A general factorizable input state has the form

\[ |\Psi_{in}^{AB}\rangle = (a_0 |0_A\rangle + a_1 |1_A\rangle) \otimes (b_0 |0_B\rangle + b_1 |1_B\rangle) \]

\[ = a_0 b_0 |0_A\rangle \otimes |0_B\rangle + a_0 b_1 |0_A\rangle \otimes |1_B\rangle + a_1 b_0 |1_A\rangle \otimes |0_B\rangle + a_1 b_1 |1_A\rangle \otimes |1_B\rangle \]

where \(|a_0|^2 + |a_1|^2 = |b_0|^2 + |b_1|^2 = 1\). If we apply \(U_{AB}\) to this state we get

\[ |\Psi_{out}^{AB}\rangle = U_{AB} |\Psi_{in}^{AB}\rangle \]

\[ = a_0 b_0 |0_A\rangle \otimes |0_B\rangle + a_0 b_1 |0_A\rangle \otimes |1_B\rangle + a_1 b_0 |1_A\rangle \otimes |0_B\rangle + a_1 b_1 |1_A\rangle \otimes |1_B\rangle \]

The simplest ways to get a maximally entangled output state are to set \(a_0 = a_1 = 1/\sqrt{2}\) and either \(b_0 = 1\) or \(b_1 = 0\). In the former case we have

\[ |\Psi_{out}^{AB}\rangle \rightarrow \frac{1}{\sqrt{2}} (|0_A\rangle \otimes |1_B\rangle + |1_A\rangle \otimes |0_B\rangle) \]

while in the latter we get

\[ |\Psi_{out}^{AB}\rangle \rightarrow \frac{1}{\sqrt{2}} (|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle) \]

In either case it is straightforward to verify that \(\text{Tr}[\hat{\rho}_A^2] = 1/2\).

### 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 \(\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B\),

\[ |\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|0_A1_B\rangle + |1_A0_B\rangle) \]

where \(|0_A1_B\rangle\) is short-hand notation for \(|0_A\rangle \otimes |1_B\rangle\) and so on. Rewrite this state in terms of a new basis \(|\tilde{0}_A0_B\rangle, |\tilde{1}_A0_B\rangle, |\tilde{1}_A1_B\rangle, |\tilde{0}_A1_B\rangle\), where

\[ |\tilde{0}_A\rangle = \cos \frac{\phi}{2} |0_A\rangle + \sin \frac{\phi}{2} |1_A\rangle \]

\[ |\tilde{1}_A\rangle = -\sin \frac{\phi}{2} |0_A\rangle + \cos \frac{\phi}{2} |1_A\rangle \]

and similarly for \(|\tilde{0}_B\rangle, |\tilde{1}_B\rangle\). Again \(|\tilde{0}_A0_B\rangle = |\tilde{0}_A\rangle \otimes |0_B\rangle\), etc. Is our particular choice of \(|\Psi_{AB}\rangle\) special in some way? We first note that

\[ |0_A\rangle = \cos \frac{\phi}{2} |\tilde{0}_A\rangle - \sin \frac{\phi}{2} |\tilde{1}_A\rangle \]

\[ |1_A\rangle = -\sin \frac{\phi}{2} |\tilde{0}_A\rangle + \cos \frac{\phi}{2} |\tilde{1}_A\rangle \]
so

\[
|0_a1_b\rangle = \left( \cos \frac{\phi}{2} |0_a\rangle - \sin \frac{\phi}{2} |1_a\rangle \right) \otimes \left( \sin \frac{\phi}{2} |0_a\rangle + \cos \frac{\phi}{2} |1_a\rangle \right)
= \sin \frac{\phi}{2} \cos \frac{\phi}{2} |0_a0_b\rangle + \cos^2 \frac{\phi}{2} |0_a1_b\rangle \\
- \sin^2 \frac{\phi}{2} |1_a0_b\rangle - \sin \frac{\phi}{2} \cos \frac{\phi}{2} |1_a1_b\rangle
\]

\[
|1_a0_b\rangle = \left( \sin \frac{\phi}{2} |0_a\rangle + \cos \frac{\phi}{2} |1_a\rangle \right) \otimes \left( \cos \frac{\phi}{2} |0_a\rangle - \sin \frac{\phi}{2} |1_a\rangle \right)
= \sin \frac{\phi}{2} \cos \frac{\phi}{2} |0_a0_b\rangle - \sin^2 \frac{\phi}{2} |0_a1_b\rangle \\
+ \cos^2 \frac{\phi}{2} |1_a0_b\rangle - \sin \frac{\phi}{2} \cos \frac{\phi}{2} |1_a1_b\rangle
\]

and

\[
|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|0_a1_b\rangle - |1_a0_b\rangle) = \frac{1}{\sqrt{2}} (|0_a\tilde{0}_b\rangle - |1_a\tilde{1}_b\rangle)
\]

From the calculations we see that it is unusual for a state to have the same expansion coefficients in the old and new basis. For example, the coefficients of \(|0_a1_b\rangle\) go from

\[
\begin{pmatrix}
0 \\
1 \\
0
\end{pmatrix}
\]

to

\[
\begin{pmatrix}
\sin \frac{\phi}{2} \cos \frac{\phi}{2} \\
\cos^2 \frac{\phi}{2} \\
-\sin^2 \frac{\phi}{2} \\
-\sin \frac{\phi}{2} \cos \frac{\phi}{2}
\end{pmatrix}
\]

### 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 \(|0_A0_B\rangle = |0_A\rangle \otimes |0_B\rangle\), etc. Let the natural tensor product basis kets for the joint space \(\mathcal{H}_{AB}\) be represented by column vectors as follows:

\[
|0_A0_B\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |0_A1_B\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1_A0_B\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |1_A1_B\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\]
For parts (a) - (c), let
\[ \rho_{AB} = \frac{3}{8} \left( |0_A\rangle \langle 0_A| \otimes \frac{1}{2} (|0_B\rangle + |1_B\rangle)(|0_B\rangle + |1_B\rangle) \
+ \frac{5}{8} |1_A\rangle \langle 1_A| \otimes \frac{1}{2} (|0_B\rangle - |1_B\rangle)(|0_B\rangle - |1_B\rangle) \right) \]

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

Expanding this out in the joint-state basis,
\[ \rho_{AB} = \frac{3}{8} |0_A\rangle \langle 0_A| \otimes \frac{1}{2} (|0_B\rangle + |1_B\rangle)(|0_B\rangle + |1_B\rangle) \
+ \frac{5}{8} |1_A\rangle \langle 1_A| \otimes \frac{1}{2} (|0_B\rangle - |1_B\rangle)(|0_B\rangle - |1_B\rangle) \]
\[ = \frac{3}{8} |0_A\rangle \langle 0_A| \otimes \frac{1}{2} (|0_B\rangle \langle 0_B| + |1_B\rangle \langle 0_B| + |0_B\rangle \langle 1_B| + |1_B\rangle \langle 1_B|) \
+ \frac{5}{8} |1_A\rangle \langle 1_A| \otimes \frac{1}{2} (|0_B\rangle \langle 0_B| - |1_B\rangle \langle 0_B| - |0_B\rangle \langle 1_B| + |1_B\rangle \langle 1_B|) \]
\[ = \frac{3}{16} (|0_a0_b\rangle \langle 0_a0_b| + |0_a1_b\rangle \langle 0_a0_b| + |0_a0_b\rangle \langle 0_a1_b| + |0_a1_b\rangle \langle 0_a1_b|) \
+ \frac{5}{16} (|1_a0_b\rangle \langle 1_a0_b| - |1_a0_b\rangle \langle 0_a0_b| - |1_a0_b\rangle \langle 0_a1_b| + |1_a1_b\rangle \langle 1_a1_b|) \]
\[ \leftrightarrow \frac{1}{16} \begin{pmatrix}
3 & 3 & 0 & 0 \\
3 & 3 & 0 & 0 \\
0 & 0 & 5 & -5 \\
0 & 0 & -5 & 5
\end{pmatrix} \]

Alternatively, we could have written
\[ \rho_{ab} = \frac{3}{16} \left( \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \right) + \frac{5}{16} \left( \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \right) \]
and gotten directly to the final answer.

(b) Find the matrix representation of the partial projectors \( I^A \otimes P_0^B \) and \( I^A \otimes P_1^B \) (see problem 6.19.18 for definitions) and then use them to compute the matrix representation of
\[ (I^A \otimes P_0^B) \rho_{AB} (I^A \otimes P_0^B) + (I^A \otimes P_1^B) \rho_{AB} (I^A \otimes P_1^B) \]

We have
\[ P_0^B \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} , \quad P_1^B \leftrightarrow \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \]

so
\[ I^A \otimes P_0^B \leftrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} , \quad I^A \otimes P_1^B \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]
Hence

\[
(I_A \otimes P_B^0) \rho_{AB} (I_A \otimes P_B^0) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix} \begin{pmatrix}
3 & 3 & 0 & 0 \\
3 & 3 & 0 & 0 \\
0 & 0 & 5 & -5 \\
0 & 0 & -5 & 5 \\
\end{pmatrix} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix}
= \frac{1}{16} \begin{pmatrix}
3 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 5 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

\[
(I_A \otimes P_B^1) \rho_{AB} (I_A \otimes P_B^1) = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
\end{pmatrix} \begin{pmatrix}
3 & 3 & 0 & 0 \\
3 & 3 & 0 & 0 \\
0 & 0 & 5 & -5 \\
0 & 0 & -5 & 5 \\
\end{pmatrix} \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
\end{pmatrix}
= \frac{1}{16} \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 3 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 5 \\
\end{pmatrix}
\]

and their sum is

\[
(I_A \otimes P_B^0) \rho_{AB} (I_A \otimes P_B^0) + (I_A \otimes P_B^1) \rho_{AB} (I_A \otimes P_B^1) \leftrightarrow \frac{1}{16} \begin{pmatrix}
3 & 0 & 0 & 0 \\
0 & 3 & 0 & 0 \\
0 & 0 & 5 & 0 \\
0 & 0 & 0 & 5 \\
\end{pmatrix}
\]

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

We start by taking the partial trace in Dirac notation:

\[
\rho_{AB} = \frac{3}{16} (|0_a0_b\rangle \langle 0_a0_b| + |0_a1_b\rangle \langle 0_a1_b| + |0_a0_b\rangle \langle 0_a1_b| + |0_a1_b\rangle \langle 0_a1_b|)
+ \frac{5}{16} (|1_a0_b\rangle \langle 1_a1_b| - |1_a0_b\rangle \langle 0_a0_b| - |1_a0_b\rangle \langle 1_a1_b| + |1_a1_b\rangle \langle 1_a1_b|)
\]

\[
\tilde{\rho}_A = \frac{3}{16} (|0_a\rangle \langle 0_a| + |0_a\rangle \langle 0_a|) + \frac{5}{16} (|1_a\rangle \langle 1_a| + |1_a\rangle \langle 1_a|)
= \frac{3}{8} |0_a\rangle \langle 0_a| + \frac{5}{8} |1_a\rangle \langle 1_a|)
\]

Thus, in matrix representation

\[
\tilde{\rho}_A = \frac{1}{8} \begin{pmatrix}
3 & 0 \\
0 & 5 \\
\end{pmatrix}
\]

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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 $|0_A0_B\rangle = |0_A\rangle \otimes |0_B\rangle$, etc. Consider the joint state

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|0_A0_B\rangle + |1_A1_B\rangle)$$

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

$$\langle \Psi_{AB} | O^A \otimes I^B | \Psi_{AB} \rangle = \langle \Psi_{AB} | (I^A \otimes P^B_0) O^A \otimes I^B (I^A \otimes P^B_0) | \Psi_{AB} \rangle$$

where

$$P^B_0 = |0^B\rangle \langle 0^B|$$

Express your answer in Dirac language.

We are looking for $O^A$ such that

$$\langle \Psi_{AB} | O^A \otimes I^B | \Psi_{AB} \rangle = \langle \Psi_{AB} | (I^A \otimes P^B_0) O^A \otimes I^B (I^A \otimes P^B_0) | \Psi_{AB} \rangle$$

$$= \langle \Psi_{AB} | (O^A I^A \otimes P^B_0 I^B P^B_0) | \Psi_{AB} \rangle$$

$$= \langle \Psi_{AB} | (O^A \otimes P^B_0) | \Psi_{AB} \rangle$$

For the specific state we are given,

$$\langle \Psi_{AB} | O^A \otimes I^B | \Psi_{AB} \rangle = \frac{1}{2} (\langle 0_A0_B| + \langle 1_A1_B|) O^A \otimes I^B (|0_A0_B\rangle + |1_A1_B\rangle)$$

$$= \frac{1}{2} (\langle 0_a| O^A |0_a\rangle + \langle 1_a| O^A |1_a\rangle)$$

$$\langle \Psi_{AB} | O^A \otimes P^B_0 | \Psi_{AB} \rangle = \frac{1}{2} (\langle 0_A0_B| + \langle 1_A1_B|) O^A \otimes P^B_0 (|0_A0_B\rangle + |1_A1_B\rangle)$$

$$= \frac{1}{2} \langle 0_a| O^A |0_a\rangle$$

Hence we simply need

$$\langle 1_a| O^A |1_a\rangle$$

The most general form of an observable for system $A$ is given in Dirac notation by

$$O^A = a |0_a\rangle \langle 0_a| + (b + ic) |0_a\rangle \langle 1_a| + (b - ic) |1_a\rangle \langle 0_a| + o_{11} |1_a\rangle \langle 1_a|$$

where $o_{00}$ and $o_{11}$ are real and $o_{10} = o_{01}^*$. The constraint we were given requires that $o_{11} = 0$, so that the most general observable has the form

$$O^A = a |0_a\rangle \langle 0_a| + (b + ic) |0_a\rangle \langle 1_a| + (b - ic) |1_a\rangle \langle 0_a| \quad a, b, c \in \mathbb{R}$$
(b) Consider the specific operator

\[ X^A = |0^A\rangle \langle 1^A| + |1^A\rangle \langle 0^A| \]

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

\[ \langle \Psi'_{AB} | X^A \otimes I^B | \Psi'_{AB} \rangle \neq \langle \Psi_{AB} | (I^A \otimes P^B_0) X^A \otimes I^B (I^A \otimes P^B_0) | \Psi_{AB} \rangle \]

The most general form of a joint state vector is

\[ |\Psi'_{AB}\rangle = c_{00} |0_A0_B\rangle + c_{01} |0_A1_B\rangle + c_{10} |1_A0_B\rangle + c_{11} |1_A1_B\rangle \]

so

\[ X^A \otimes I^B |\Psi'_{AB}\rangle = c_{00} (|0_a\rangle \langle 1_a| + |1_a\rangle \langle 0_a|) |0_A0_B\rangle + c_{01} (|0_a\rangle \langle 1_a| + |1_a\rangle \langle 0_a|) |0_A1_B\rangle \\
+ c_{10} (|0_a\rangle \langle 1_a| + |1_a\rangle \langle 0_a|) |1_A0_B\rangle + c_{11} (|0_a\rangle \langle 1_a| + |1_a\rangle \langle 0_a|) |1_A1_B\rangle \]

\[ = c_{00} (I_a) \otimes |0_b\rangle + c_{01} (I_a) \otimes |1_b\rangle + c_{10} (0_a) \otimes |0_b\rangle + c_{11} (0_a) \otimes |1_b\rangle \]

\[ = c_{10} |0_a0_b\rangle + c_{11} |0_a1_b\rangle + c_{00} |1_a0_b\rangle + c_{01} |1_a1_b\rangle \]

and

\[ \langle \Psi'_{AB} | X^A \otimes I^B | \Psi'_{AB} \rangle = c_{00}^* c_{10} + c_{01}^* c_{11} + c_{10}^* c_{00} + c_{11}^* c_{11} \]

\[ = 2 \text{Re}[c_{00}^* c_{10} + c_{01}^* c_{11}] \]

With the projected form, however,

\[ (I^A \otimes P^B_0) |\Psi'_{AB}\rangle = c_{00} |0_A0_b\rangle + c_{10} |1_A0_b\rangle \]

and

\[ X^A \otimes I^B (I^A \otimes P^B_0) |\Psi'_{AB}\rangle = c_{00} (|0_a\rangle \langle 1_a| + |1_a\rangle \langle 0_a|) |0_A0_b\rangle \\
+ c_{10} (|0_a\rangle \langle 1_a| + |1_a\rangle \langle 0_a|) |1_A0_b\rangle \]

\[ = (c_{00} |1_a\rangle + c_{10} |0_a\rangle) |0_b\rangle \]

so

\[ \langle \Psi_{AB} | X^A \otimes I^B (I^A \otimes P^B_0) | \Psi'_{AB} \rangle = c_{00}^* c_{10} + c_{10}^* c_{00} \]

\[ = 2 \text{Re}[c_{00}^* c_{10}] \]

Comparing the two results, we only need \( \text{Re}[c_{00}^* c_{10}] \neq 0 \).

(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

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

We have

\[ |\Psi'_{AB}\rangle = c_{00} |0_A0_B\rangle + c_{01} |0_A1_B\rangle + c_{10} |1_A0_B\rangle + c_{11} |1_A1_B\rangle \]
\[
\langle \Psi_{AB}' \rangle = c_{00}^* \langle 0_A 0_B | + c_{01}^* \langle 0_A 1_B | + c_{10}^* \langle 1_A 0_B | + c_{11}^* \langle 1_A 1_B |
\]

together with the constraint \( \text{Re}[c_{00} c_{10}] \neq 0 \). We compute
\[
|\Psi_{AB}'\rangle \langle \Psi_{AB}'| = c_{00} |0_A 0_B \rangle \langle 0_A 0_B | + c_{01} |0_A 1_B \rangle \langle 0_A 1_B | + c_{10} |1_A 0_B \rangle \langle 1_A 0_B | + c_{11} |1_A 1_B \rangle \langle 1_A 1_B | + c_{01} |0_A 1_B \rangle \langle 0_A 1_B | + c_{10} |1_A 0_B \rangle \langle 1_A 0_B | + c_{11} |1_A 1_B \rangle \langle 1_A 1_B |
\]

and
\[
\hat{\rho}_A = Tr_B |\Psi_{AB}'\rangle \langle \Psi_{AB}'|
\]

\[
= c_{00} |0_A \rangle \langle 0_a | + c_{01} |0_A \rangle \langle 0_1 | + c_{10} |1_A \rangle \langle 0_1 | + c_{11} |1_A \rangle \langle 1_1 | + |0_A \rangle \langle 0_a | + c_{01} |0_1 | + c_{10} |1_1 | + |1_A \rangle \langle 1_a |
\]

\[
= (|c_{00}|^2 + |c_{01}|^2) |0_A \rangle \langle 0_a | + (c_{00} c_{01}^* + c_{01} c_{10}^*) |0_A \rangle \langle 0_1 | + (c_{10} c_{00}^* + c_{11} c_{01}^*) |1_A \rangle \langle 0_a | + (|c_{10}|^2 + |c_{11}|^2) |1_A \rangle \langle 1_a |.
\]

Since we require \( \text{Re}[c_{00} c_{10}] \neq 0 \), it follows that \( |c_{11}|^2 > 0 \). It then becomes clear that, for example, we cannot achieve
\[
\hat{\rho}_A |0_a \rangle \langle 0_a |
\]

since this would require \( |c_{00}|^2 + |c_{01}|^2 = 1 \), but by normalization \( |c_{00}|^2 + |c_{01}|^2 \leq 1 - |c_{11}|^2 \).

### 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
\[
|\Psi_{AB}^0\rangle = \frac{1}{\sqrt{2}} (|0_A 0_B \rangle + |1_A 1_B \rangle)
\]

(a) Suppose you take the \( A \) and \( B \) systems prepared in the state \( |\Psi_{AB}^0\rangle \) 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(probability \( p \)) the result of the procedure performed by your friend is the state
\[
\frac{1}{\sqrt{2}} (|0_a 0_b \rangle - |1_a 1_b \rangle)
\]

and if the result is a tail(probability \( 1 - p \)) the result of the procedure performed by your friend is the state
\[
\frac{1}{\sqrt{2}} (|0_a 0_b \rangle + |1_a 1_b \rangle)
\]

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i.e., nothing happened. After this procedure what is the density operator you should use to represent your knowledge of the joint state? We now have a mixed ensemble

\[ p : \ket{\Psi_{AB}^{\text{out}}}_A = \frac{1}{\sqrt{2}}(|0_a0_b\rangle - |1_a1_b\rangle) \]

\[ 1-p : \ket{\Psi_{AB}^{\text{out}}}_A = \frac{1}{\sqrt{2}}(|0_a0_b\rangle + |1_a1_b\rangle) \]

The corresponding density operator is

\[ \rho_{AB} = \frac{p}{2} (|0_A0_B\rangle \langle 0_A0_B| - |0_A0_B\rangle \langle 0_A0_B| + |1_A1_B\rangle \langle 0_A0_B| + |1_A1_B\rangle \langle 1_A1_B|) + \frac{1-p}{2} (|0_A0_B\rangle \langle 0_A0_B| + |0_A0_B\rangle \langle 1_A1_B| + |1_A1_B\rangle \langle 0_A0_B| + |1_A1_B\rangle \langle 1_A1_B|) \]

\[ = -p (|0_A0_B\rangle \langle 0_A0_B| + |1_A1_B\rangle \langle 0_A0_B|) + \frac{1}{2} (|0_A0_B\rangle \langle 0_A0_B| + |0_A0_B\rangle \langle 1_A1_B| + |1_A1_B\rangle \langle 0_A0_B| + |1_A1_B\rangle \langle 1_A1_B|) \]

\[ = \frac{1}{2} (|0_A0_B\rangle \langle 0_A0_B| + |0_A0_B\rangle \langle 0_A0_B|) + \frac{1-2p}{2} (|0_A0_B\rangle \langle 1_A1_B| + |1_A1_B\rangle \langle 0_A0_B|) \]

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

\[ O = I^A \otimes (|0_B\rangle \langle 0_B| - |1_B\rangle \langle 1_B|) \]

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).

The given form of \( O \) already specifies its spectral decomposition:

\[ O = (+1)(I^A \otimes |0_b\rangle \langle 0_b|) + (-1)(I^A \otimes |1_b\rangle \langle 1_b|) \]

It is easy to see that the two possible outcomes of the measurement \((\pm 1)\) are equally likely. using the projection postulate we can associate

\[ +1 : \ket{\Psi_{AB}^0} \frac{(I^A \otimes |0_b\rangle \langle 0_b|) \ket{\Psi_{AB}^0}}{\sqrt{\langle \Psi_{AB}^0 | (I^A \otimes |0_b\rangle \langle 0_b|) \ket{\Psi_{AB}^0}}} = |0_A0_B\rangle \]

\[ -1 : \ket{\Psi_{AB}^0} \frac{(I^A \otimes |1_b\rangle \langle 1_b|) \ket{\Psi_{AB}^0}}{\sqrt{\langle \Psi_{AB}^0 | (I^A \otimes |1_b\rangle \langle 1_b|) \ket{\Psi_{AB}^0}}} = |1_A1_B\rangle \]

so we can simply set

\[ \rho_{AB} = \frac{1}{2} |0_A0_B\rangle \langle 0_A0_B| + \frac{1}{2} |1_A1_B\rangle \langle 1_A1_B| \]
6.19.24 Complete Sets of Commuting Observables

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

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

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.

First we check which observables commute.

$$[O_\alpha, O_\beta] = O_\alpha O_\beta - O_\beta O_\alpha$$

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

Likewise,

$$[O_\alpha, O_\gamma] = O_\alpha O_\gamma - O_\gamma O_\alpha$$

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

Finally,

$$[O_\beta, O_\gamma] = O_\beta O_\gamma - O_\gamma O_\beta$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0$$
We conclude that the possible CSCO’s are \{O_\alpha\}, \{O_\beta\}, \{O_\gamma\}, \{O_\alpha, O_\beta\} and \{O_\beta, O_\gamma\}. We next check the eigenvalues.

\[
O_\alpha : 0 = \det \begin{pmatrix} 1 - \lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix}
\]

\[
\rightarrow \lambda^2(1 - \lambda) = \lambda(1 - \lambda) + 1 = 0
\]

so we have \(\lambda = 0\) and the roots of \(\lambda^2 - \lambda - 1 = 0\) which are

\[
\lambda = \frac{1}{2} \pm \frac{\sqrt{5}}{2}
\]

Hence, we see that all three eigenvalues are distinct and \{O_\alpha\} is OK on its own!. This also means that \{O_\alpha, O_\beta\} is automatically a valid CSCO.

The matrix forms of \(O_\beta\) and \(O_\gamma\) make it clear that each of these observables has eigenvalues 0 and 1, with the latter having two-fold degeneracy. Hence, neither \{O_\beta\} nor \{O_\gamma\} is OK on its own.

Finally, we note that the three obvious basis vectors have distinct pairs of eigenvalues for \(O_\beta\) and \(O_\gamma\):

\[
\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} : (1, 0), \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} : (1, 1), \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} : (0, 1)
\]

So, finally, the valid CSCO’s are \{O_\alpha\}, \{O_\alpha, O_\beta\}, and \{O_\beta, O_\gamma\}.

**6.19.25 Conserved Quantum Numbers**

Determine which of the CSCO’s in problem 6.19.24 (if any) are conserved by the Schrodinger equation with Hamiltonian

\[
H = \varepsilon_0 \begin{pmatrix} 2 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \varepsilon_0 (O_\alpha) + (O_\beta)
\]

Since the criterion for this is that each of the observables in the CSCO should commute with the Hamiltonian, we simply check (using the results from 6.19.24)

\[
[O_\alpha, H] = \varepsilon_0 [O_\alpha, O_\alpha + O_\beta] = 0
\]

\[
[O_\beta, H] = \varepsilon_0 [O_\beta, O_\alpha + O_\beta] = 0
\]

\[
[O_\gamma, H] = \varepsilon_0 [O_\gamma, O_\alpha + O_\beta] = \varepsilon_0 [O_\gamma, O_\alpha + O_\beta] = \varepsilon_0 [O_\gamma, O_\alpha] + \varepsilon_0 [O_\gamma, O_\beta] = 0
\]

Hence, only \{O_\alpha\} and \{O_\alpha, O_\beta\} are conserved.
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 \{\ket{x}, \ket{y}\} basis.

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

We have
\[
\ket{R} = \frac{1}{\sqrt{2}} (\ket{x} + i \ket{y}), \quad \ket{L} = \frac{1}{\sqrt{2}} (\ket{x} - i \ket{y})
\]
\[
\ket{45^\circ} = \frac{1}{\sqrt{2}} (\ket{x} + \ket{y}), \quad \ket{135^\circ} = \frac{1}{\sqrt{2}} (- \ket{x} + \ket{y})
\]

Therefore, inverting we have
\[
\ket{x} = \bra{R} \ket{x} \bra{x} \ket{R} + \bra{L} \ket{x} \bra{x} \ket{L} = \frac{1}{\sqrt{2}} (\ket{R} + \ket{L})
\]
\[
\ket{y} = \bra{R} \ket{y} \bra{y} \ket{R} + \bra{L} \ket{y} \bra{y} \ket{L} = \frac{1}{\sqrt{2}} (- \ket{R} + \ket{L})
\]

and
\[
\ket{x} = \bra{45^\circ} \ket{x} \bra{x} \ket{45^\circ} + \bra{135^\circ} \ket{x} \bra{x} \ket{135^\circ} = \frac{1}{\sqrt{2}} (\ket{45^\circ} + \ket{135^\circ})
\]
\[
\ket{y} = \bra{45^\circ} \ket{y} \bra{y} \ket{45^\circ} + \bra{135^\circ} \ket{y} \bra{y} \ket{135^\circ} = \frac{1}{\sqrt{2}} (- \ket{45^\circ} + \ket{135^\circ})
\]

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

We have
\[
\hat{P}_{\text{vert}} = \hat{P}_y = \ket{y} \bra{y}
\]
In the (R,L) basis, we have
\[
\hat{P}_y = \begin{pmatrix}
\langle R \mid y \rangle \langle y \mid R \rangle & \langle R \mid y \rangle \langle y \mid L \rangle \\
\langle L \mid y \rangle \langle y \mid R \rangle & \langle L \mid y \rangle \langle y \mid L \rangle
\end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}
\]
which can also be seen from
\[
\hat{P}_{\text{vert}} = \hat{P}_y = |y \rangle \langle y | = \left( \frac{i}{\sqrt{2}} (-|R\rangle + |L\rangle) \right) \left( \frac{-i}{\sqrt{2}} (-|R\rangle + \langle L|) \right)
= \frac{1}{2} (|R\rangle \langle R| - |R\rangle \langle L| - |L\rangle \langle R| + |L\rangle \langle L|)
\]

### 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.

We have
\[
|\theta\rangle = \cos \theta |x\rangle + \sin \theta |y\rangle
\]
\[
|30\rangle = \frac{\sqrt{3}}{2} |x\rangle + \frac{1}{2} |y\rangle
\]
\[
|45\rangle = \frac{1}{\sqrt{2}} |x\rangle + \frac{1}{\sqrt{2}} |y\rangle
\]
\[
|60\rangle = \frac{1}{2} |x\rangle + \frac{\sqrt{3}}{2} |y\rangle
\]

Then
\[
P(x \rightarrow 45 \rightarrow y) = |\langle y \mid y \rangle \langle y \mid 45 \rangle \langle 45 \mid x \rangle|^2 = \frac{1}{4}
\]

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.

\[
P(x \rightarrow 30 \rightarrow 60 \rightarrow y) = |\langle y \mid y \rangle \langle y \mid 60 \rangle \langle 60 \mid 30 \rangle \langle 30 \mid x \rangle|^2
= |(y \mid 60 \rangle \langle 60 \mid 30 \rangle \langle 30 \mid x \rangle|^2
= \frac{\sqrt{3} \sqrt{3} \sqrt{3}}{2 \cdot 2 \cdot 2} = \frac{27}{64}
\]
7.5.3 Calcite Crystal

A photon polarized at an angle $\theta$ to the optic axis is sent through a slab of calcite crystal. Assume that the slab is $10^{-2} \text{cm}$ 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 $\theta$, the transition probability for the photon to emerge left circularly polarized. Sketch the result. Let the frequency of the light be given by $c/\omega = 5000 \text{Å}$, and let $n_e = 1.50$ and $n_o = 1.65$ for the calcite indices of refraction.

We have

$$|in\rangle = \cos \theta |o\rangle + \sin \theta |e\rangle$$

$$|out\rangle = \hat{T} |in\rangle = (e^{ik_o\ell} |o\rangle + e^{ik_e\ell} |e\rangle) |in\rangle$$

$$|\text{final}\rangle = |L\rangle = \frac{1}{\sqrt{2}} (|o\rangle - i|e\rangle)$$

$$P = \text{probability of emerging LCP (in |L\rangle state)} = |\langle L | out\rangle|^2$$

$$P = \frac{1}{2} |e^{ik_e \ell} \cos \theta + ie^{ik_e \ell} \sin \theta|^2 = \frac{1}{2} (1 + \sin 2\theta \sin (k_o - k_e) \ell)$$

Now

$$\ell = 10^{-2} \text{cm} \quad , \quad \frac{\omega}{c} = 5000 \frac{\text{Å}}{\text{cm}} = 5 \times 10^{-5} \text{ cm}$$

$$n_e = 1.50 \rightarrow k_e \ell = \frac{c}{n_e} \ell = 300$$

$$n_o = 1.65 \rightarrow k_o \ell = \frac{c}{n_o} \ell = 330$$

$$\sin (k_o - k_e) \ell = \sin 30 = -0.9880$$

so that

$$P = \frac{1}{2} (1 - 0.988 \sin 2\theta)$$

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.

We have

$$|out\rangle = R(\theta) |in\rangle$$

where

$$R(\theta) = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} = \text{rotation operator}$$
Proof:

\[ R(\theta) |\varphi\rangle = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \cos \varphi \\ \sin \varphi \end{pmatrix} = \begin{pmatrix} \cos \varphi \cos \theta + \sin \theta \sin \varphi \\ -\sin \theta \cos \varphi + \cos \theta \sin \varphi \end{pmatrix} = \begin{pmatrix} \cos(\varphi - \theta) \\ \sin(\varphi - \theta) \end{pmatrix} = |\varphi - \theta\rangle \]

and

\[ \theta = -\frac{\pi \ell}{36} \rightarrow 5^\circ \text{ per cm} \]

Since \( R^+ R = I \rightarrow R^+ = R^{-1} \rightarrow R \) is unitary

It is important that the operator be unitary since it will preserve the length of the vector and also the probability interpretation of the length-squared.

The eigenvectors are \(|RCP\rangle\) and \(|LCP\rangle\) with eigenvalues \(e^{i\theta}\) and \(e^{-i\theta}\).

Proof:

\[
\begin{align*}
\det \begin{pmatrix} \cos \theta - \lambda & \sin \theta \\ -\sin \theta & \cos \theta - \lambda \end{pmatrix} &= 0 = (\cos \theta - \lambda)^2 + \sin^2 \theta \\
0 &= \cos^2 \theta + \sin^2 \theta - 2\lambda \cos \theta + \lambda^2 = \lambda^2 - 2\lambda \cos \theta + 1 \\
\lambda &= \frac{2 \cos \theta \pm \sqrt{4 \cos^2 \theta - 4}}{2} = \cos \theta \pm i \sin \theta = e^{\pm i\theta}
\end{align*}
\]

\[
\begin{align*}
a_\pm &\cos \theta + b_\pm \sin \theta = a_\pm \cos \theta \pm ia_\pm \sin \theta \\
b_\pm &= \pm ia_\pm
\end{align*}
\]

\[
|e^{\pm i\theta}\rangle = a_\pm \begin{pmatrix} 1 \\ \pm i \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix}
\]

\[
|e^{i\theta}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} = |R\rangle, \quad |e^{-i\theta}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} = |L\rangle
\]

In general, we can write

\[ |in\rangle = |R\rangle \langle R | in\rangle + |L\rangle \langle L | in\rangle \]

so that

\[ |out\rangle = R(\theta) |in\rangle = R(\theta) |R\rangle \langle R | in\rangle + R(\theta) |L\rangle \langle L | in\rangle = e^{i\theta} |R\rangle \langle R | in\rangle + e^{-i\theta} |L\rangle \langle L | in\rangle = e^{-i\frac{\pi \ell}{36}} |R\rangle \langle R | in\rangle + e^{-i\frac{\pi \ell}{36}} |L\rangle \langle L | in\rangle \]

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.

We have

\[
|\text{in}\rangle = R(\theta) |x\rangle = \cos \theta |x\rangle + \sin \theta |y\rangle, \quad \theta = 30^\circ
\]

\[
P_{Ry} = |\langle y | R \rangle \langle R | \text{in}\rangle|^2 = \text{probability of } |\text{out}\rangle = |y\rangle \text{ via } |R\rangle
\]

\[
P_{Ly} = |\langle y | L \rangle \langle L | \text{in}\rangle|^2 = \text{probability of } |\text{out}\rangle = |y\rangle \text{ via } |L\rangle
\]

\[
P_y = |\langle y | \text{in}\rangle|^2 = |\langle y | R \rangle \langle R | \text{in}\rangle + \langle y | L \rangle \langle L | \text{in}\rangle|^2
\]

where

\[
\langle y | R \rangle \langle R | \text{in}\rangle = \text{amplitude for } |\text{out}\rangle = |y\rangle \text{ via } |R\rangle
\]

\[
\langle y | L \rangle \langle L | \text{in}\rangle = \text{amplitude for } |\text{out}\rangle = |y\rangle \text{ via } |L\rangle
\]

We then have

\[
P_y = P_{Ry} + P_{Ly} + 2\text{Real} \left( \langle y | R \rangle \langle R | \text{in}\rangle \right) \ast \left( \langle y | L \rangle \langle L | \text{in}\rangle \right)
\]

Now,

\[
\langle R | \text{in}\rangle = \frac{1}{\sqrt{2}}, \quad \langle y | L \rangle = -\frac{1}{\sqrt{2}}
\]

\[
\langle R | \text{in}\rangle = \langle R | R(\theta) |x\rangle = e^{-i\theta} \langle R | x \rangle = \frac{1}{\sqrt{2}} e^{-i\theta}
\]

\[
\langle L | \text{in}\rangle = \langle L | R(\theta) |x\rangle = e^{i\theta} \langle L | x \rangle = \frac{1}{\sqrt{2}} e^{i\theta}
\]

so that

\[
P_{Ry} = \frac{1}{4} = P_{Ly} \rightarrow P_{Ry} + P_{Ly} = \frac{1}{2} = \text{classical probability result}
\]

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and
\[ P_y = \frac{1}{4} + \frac{1}{4} + 2\text{Real} \left( \left( \frac{i}{\sqrt{2}} - \frac{1}{\sqrt{2}} e^{-i\theta} \right)^* \left( -\frac{i}{\sqrt{2}} \sqrt{2} e^{i\theta} \right) \right) = \frac{1}{2}(1 - \cos 2\theta) \]

is the quantum mechanical result. For \( \theta = 30^\circ \) we have \( P_y = 1/2 = \text{quantum result, which is clearly different.} \)

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

We have
\[
\hat{\rho}_\text{in} = |\text{in}\rangle \langle \text{in}|, \quad |\text{in}\rangle = \frac{\sqrt{3}}{2} |x\rangle + \frac{1}{2} |y\rangle = \frac{1}{2\sqrt{2}} \left( (\sqrt{3} + i) |R\rangle + (\sqrt{3} - i) |L\rangle \right)
\]

so that
\[
\hat{\rho}_\text{in} = \frac{3}{4} |x\rangle \langle x| + \frac{\sqrt{3}}{4} |x\rangle \langle y| + \frac{\sqrt{3}}{4} |y\rangle \langle x| + \frac{1}{4} |y\rangle \langle y|
\]
\[
= \frac{3}{4} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{\sqrt{3}}{4} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \frac{\sqrt{3}}{4} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 3 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}
\]

Since
\[ \text{Prob}(j) = Tr(\hat{P}_j \hat{\rho}) = Tr(|j\rangle \langle j| \hat{\rho}) = \sum_k \langle k| |j\rangle \langle j| \hat{\rho} |k\rangle = \sum_k \delta_{kj} \langle j| \hat{\rho} |k\rangle = \hat{\rho}_{jj} \]

we have
\[ \text{Prob}(x) = \frac{3}{4}, \quad \text{Prob}(y) = \frac{1}{4} = \text{quantum result} \]

Alternatively, we can think of a measurement taking place in the \( xy \) basis. This measurement cannot be done in the quantum world without destroying the phase relationships and hence eliminating any interference effects, that is, measurement separates orthogonal states making them classically distinct and all interference between orthogonal states (represented by the off-diagonal terms in \( \hat{\rho} \)) is destroyed.

Simply put: measurement diagonalizes \( \hat{\rho} \) in the basis of the measurement!

So
\[ \frac{1}{4} \begin{pmatrix} 3 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix} \rightarrow \frac{1}{4} \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix} \]

so that
\[ \text{Prob}(x) = \frac{3}{4}, \quad \text{Prob}(y) = \frac{1}{4} = \text{as before} \]

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To see what happens if we attempt to find out whether the photons are passing through the apparatus as $R$ or $L$ photons, we must first rewrite $\hat{\rho}_{in}$ in the $(R,L)$ basis, so that

$$\hat{\rho}_{in} = \frac{1}{2} |R\rangle \langle R| + \frac{1 + \sqrt{3}i}{8} |R\rangle \langle L| + \frac{1 - \sqrt{3}i}{8} |L\rangle \langle R| + \frac{1}{2} |L\rangle \langle L|$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1 + \sqrt{3}i}{8} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \frac{1 - \sqrt{3}i}{8} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \frac{1}{8} \begin{pmatrix} 4 & 1 - \sqrt{3}i \\ 1 + \sqrt{3}i & 4 \end{pmatrix}_{RL}$$

which implies that

$$Prob(R) = \frac{1}{2}, \quad Prob(L) = \frac{1}{2} = \text{quantum result}$$

Now we measure in the $(R, L)$ basis (since we are trying to determine if the photon passes through the apparatus as a $R$ or $L$ photon). Again, this measurement cannot be done in the quantum world without destroying the phase relationships and hence eliminating any interference effects, that is, measurement separates orthogonal states making them classically distinct and all interference between orthogonal states (represented by the off-diagonal terms in $\hat{\rho}$) is destroyed.

Simply put again: measurement diagonalizes $\hat{\rho}$ in the basis of the measurement!

So

$$\hat{\rho}_{in} = \frac{1}{8} \begin{pmatrix} 4 & 1 - \sqrt{3}i \\ 1 + \sqrt{3}i & 4 \end{pmatrix}_{RL} \rightarrow \hat{\rho}_{out} = \frac{1}{8} \begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}_{RL}$$

Measurement has changed $\hat{\rho}_{out}$ to

$$\hat{\rho}_{out} = \frac{1}{2} |R\rangle \langle R| + \frac{1}{2} |L\rangle \langle L| \rightarrow \text{a mixed state}$$

Changing back to the $xy$ basis we get

$$\hat{\rho}_{out} = \frac{1}{2} \frac{1}{2} (|x\rangle + i |y\rangle) (|x\rangle - i |y\rangle) + \frac{1}{2} \frac{1}{2} (|x\rangle - i |y\rangle) (|x\rangle + i |y\rangle)$$

$$= \frac{1}{2} |x\rangle \langle x| + \frac{1}{2} |y\rangle \langle y| = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_{xy} \rightarrow \text{a mixed state}$$

The density operator remains diagonal!

Clearly,

$$Prob(x) = \frac{1}{2}, \quad Prob(y) = \frac{1}{2} = \text{classical result}$$
The measurement turns pure states into mixed states with coefficients equal to measurement probabilities!

This problem is the same as the two-slit diffraction experiment if one tries to determine which slit the photon went through - that measurement will destroy the interference pattern!

### 7.5.6 Photons and Polarizers

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

$$|\psi\rangle = \sqrt{\frac{2}{3}}|x\rangle + i \sqrt{\frac{1}{3}}|y\rangle$$

(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?

$$\langle x | \psi \rangle = i \sqrt{\frac{1}{3}} \rightarrow P_y = |\langle x | \psi \rangle|^2 = \frac{1}{3}$$

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

$$|y'\rangle = -\sin \varphi |x\rangle + \cos \varphi |y\rangle$$

$$\langle y' | \psi \rangle = -i \sqrt{\frac{2}{3}} \sin \varphi + i \sqrt{\frac{1}{3}} \cos \varphi$$

$$P_{y'} = |\langle y' | \psi \rangle|^2 = \frac{2}{3} \sin^2 \varphi + \frac{1}{3} \cos^2 \varphi = \frac{1}{3} (2 - \cos^2 \varphi)$$

(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.

$$|R\rangle = \frac{1}{\sqrt{2}}(|x\rangle + i |y\rangle) \rightarrow \langle R | \psi \rangle = \frac{1}{\sqrt{3}}\left(1 + \frac{\sqrt{2}}{2}\right)$$

$$P_R = |\langle R | \psi \rangle|^2 = \frac{1}{2} + \frac{\sqrt{2}}{3} \rightarrow P_L = 1 - P_R = \frac{1}{2} - \frac{\sqrt{2}}{3}$$

The torque on the disk is the angular momentum transferred per second, which is

\[
\text{amount transferred by } |R\rangle \text{ per sec} + \text{amount transferred by } |L\rangle \text{ per sec}
\]

or

\[
N (\hbar P(R) - \hbar P(-L)) \quad N (\hbar P(R) - \hbar P(L))
\]

\[
N\hbar \left(\frac{1}{2} + \frac{\sqrt{2}}{3}\right) - N\hbar \left(\frac{1}{2} - \frac{\sqrt{2}}{3}\right) = 2\sqrt{2}\hbar N
\]

Thus, the torque is positive, which implies that the disk will rotate CCW as viewed from the positive $z$-axis.
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?

The eigenvalue equation is $\hat{H} |E\rangle = E |E\rangle$ or

$$
\begin{pmatrix}
0 & -iE_0 \\
iE_0 & 0
\end{pmatrix}
\begin{pmatrix}
\langle x | E \rangle \\
\langle y | E \rangle
\end{pmatrix}
= E
\begin{pmatrix}
\langle x | E \rangle \\
\langle y | E \rangle
\end{pmatrix}
$$

which will have a non-trivial solution only if

$$
\begin{vmatrix}
-E & -iE_0 \\
iE_0 & -E
\end{vmatrix}
= 0 = E^2 - E_0^2 \rightarrow E = \pm E_0 = \text{eigenvalues}
$$

For $E = +E_0$, we get

$$
\langle y | E_0 \rangle = i \langle x | E_0 \rangle \rightarrow |E_0\rangle = \frac{1}{\sqrt{2}} (|x\rangle + i |y\rangle) = |R\rangle
$$

and for $E = -E_0$, we get

$$
\langle y | -E_0 \rangle = -i \langle x | -E_0 \rangle \rightarrow |-E_0\rangle = \frac{1}{\sqrt{2}} (|x\rangle - i |y\rangle) = |L\rangle
$$

Thus, the eigenvectors are the RCP and LCP photon states.

(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.

We have

$$
|\psi(0)\rangle = |in\rangle = |x\rangle = |E_0\rangle \langle E_0 | x\rangle + |-E_0\rangle \langle -E_0 | x\rangle = \frac{1}{\sqrt{2}} (|E_0\rangle + |-E_0\rangle)
$$

This implies that

$$
|\text{out}\rangle = e^{-i\hat{H}t/\hbar} |\text{in}\rangle = e^{-i\hat{H}t/\hbar} \frac{1}{\sqrt{2}} (|E_0\rangle + |-E_0\rangle) = \frac{1}{\sqrt{2}} \left( e^{-iE_0t/\hbar} |E_0\rangle + e^{iE_0t/\hbar} |-E_0\rangle \right)
$$

$$
= \cos \left( \frac{E_0t}{\hbar} \right) |x\rangle + \sin \left( \frac{E_0t}{\hbar} \right) |y\rangle = |\psi(t)\rangle
$$
(c) What is happening to the polarization of the photon as it travels through the crystal?

Since a linearly polarized state with polarization along \( x' \) is given by
\[
|x'\rangle = \cos \varphi |x\rangle + \sin \varphi |y\rangle
\]
we see that \( |\psi(t)\rangle \) corresponds to a linearly polarized photon state whose direction of polarization
\[
\varphi = \frac{E_0 t}{\hbar}
\]
rotates as the photon propagates 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
\[
|K_L(t)\rangle = e^{-i\omega_L t - t/2\tau_L} |K_L\rangle \quad \text{and} \quad |K_S(t)\rangle = e^{-i\omega_S t - t/2\tau_S} |K_S\rangle
\]
where
\[
\omega_L = \frac{E_L}{\hbar}, \quad E_L = \left( p^2 c^2 + m_L^2 c^4 \right)^{1/2} \\
\omega_S = \frac{E_S}{\hbar}, \quad E_S = \left( p^2 c^2 + m_S^2 c^4 \right)^{1/2}
\]
and
\[
\tau_S \approx 0.9 \times 10^{-10} \text{ sec}, \quad \tau_L \approx 560 \times 10^{-10} \text{ sec}
\]
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 \( = mc \).

Before the absorber we have the state
\[
|\psi_{\text{before}}\rangle = |K_L\rangle = \frac{1}{\sqrt{2}} \left( |K^0\rangle - |\bar{K}^0\rangle \right)
\]
The effect of the thin absorber is expressed by the development operator
\[
\hat{A} = |K^0\rangle \langle K^0| e^{i\theta} + |\bar{K}^0\rangle \langle \bar{K}^0| e^{i(\theta + \pi/18)}
\]
so that only the relative phase of the components is changed by 10° = \( \pi/18 \). Therefore, after the absorber the state is
\[
|\psi_{\text{after}}\rangle = \hat{A} |\psi_{\text{before}}\rangle = \frac{e^{i\theta}}{\sqrt{2}} \left( |K^0\rangle - e^{i\pi/18} |\bar{K}^0\rangle \right)
\]
We know the time dependence of the $|K_L\rangle, |K_S\rangle$ states so we now rewrite this state in that basis

$$|\psi_{\text{after}}\rangle = \frac{e^{i\theta}}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} (|K_S\rangle + |K_L\rangle) - e^{i\pi/18} \frac{1}{\sqrt{2}} (|K_S\rangle - |K_L\rangle) \right)$$

$$= \frac{e^{i\theta}}{2} \left( (1 - e^{i\pi/18}) |K_S\rangle + (1 + e^{i\pi/18}) |K_L\rangle \right)$$

This is the state at $t = 0$, $|\psi(0)\rangle$, or just after leaving the absorber. The $|K_L\rangle, |K_S\rangle$ states have this time dependence (they change phase and decay as the beam travels in the laboratory)

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

Therefore, for $t > 0$, we have

$$|\psi(t)\rangle = \frac{e^{i\theta}}{2} \left( (1 - e^{i\pi/18}) e^{-i\omega_S t - t/2\tau_S} |K_S\rangle + (1 + e^{i\pi/18}) e^{-i\omega_L t - t/2\tau_L} |K_L\rangle \right)$$

The probability amplitude for observing $|K_S\rangle$ for $t > 0$ is

$$\langle K_S | \psi(t) \rangle = \frac{e^{i\theta}}{2} \left( 1 - e^{i\pi/18} \right) e^{-i\omega_S t - t/2\tau_S}$$

and the corresponding probability is

$$P_S = |\langle K_S | \psi(t) \rangle|^2 = \frac{1}{2} \left( 1 - \cos \frac{\pi}{18} \right) e^{-t/\tau_S}$$

Note that for $\pi/18 \rightarrow 0$ or no relative phase shift, the probability $= 0$, that is, the beam stays all $|K_L\rangle$ as it should.

Now we have

$$d = 5 \text{ cm} \rightarrow t_d = \frac{d}{v} \approx \frac{d}{c} = 1.6 \times 10^{-10} \text{ sec}$$
$$\tau_S = 0.9 \times 10^{-10} \text{ sec} \rightarrow t_d/\tau_S = \frac{16}{9}$$

Now the number of transitions per sec at time $t$ is given by $N(0)P_S(t)$. This says that the

$$\text{total number of transitions}(0 \rightarrow t_d) = \bar{N} = \int_0^{t_d} N(0)P_S(t)dt$$

$$\bar{N} = \frac{1}{2} \left( 1 - \cos \frac{\pi}{18} \right) N(0) \int_0^{t_d} e^{-t/\tau_S} dt = \frac{1}{2} \left( 1 - \cos \frac{\pi}{18} \right) \tau_S N(0)(1-e^{-16/9}) = 0.0063 \tau_S N(0)$$

where we assumed $N(0) = \text{constant}$ since the total number of decays is very small compared to $N(0)$. Therefore,

$$\text{fraction} = \frac{\bar{N}}{N(0)} = 0.0063 \tau_S = 5.69 \times 10^{-13}$$
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 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 $\theta$ 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?

We use the $\hat{S}_z$ diagonal basis $|\pm\hat{z}\rangle$. The first measurement corresponds to the projection operator

$$\hat{M}(+\hat{z}) = |+\hat{z}\rangle \langle +\hat{z}|$$

The second measurement is given by the projection operator

$$\hat{M}(+\hat{n}) = |+\hat{n}\rangle \langle +\hat{n}|$$

where

$$|+\hat{n}\rangle = \cos \frac{\theta}{2} |+\hat{z}\rangle + \sin \frac{\theta}{2} |\hat{z}\rangle$$

so that

$$\hat{M}(+\hat{n}) = \cos^2 \frac{\theta}{2} |+\hat{z}\rangle \langle +\hat{z}| + \cos \frac{\theta}{2} \sin \frac{\theta}{2} (|+\hat{z}\rangle \langle -\hat{z}| + |\hat{z}\rangle \langle +\hat{z}|) + \sin^2 \frac{\theta}{2} |\hat{z}\rangle \langle \hat{z}|$$

The last measurement corresponds to the projection operator

$$\hat{M}(-\hat{z}) = |--\hat{z}\rangle \langle -\hat{z}|$$

The total or combined measurement is given by the product in the appropriate order

$$\hat{M}_T = \hat{M}(-\hat{z})\hat{M}(+\hat{n})\hat{M}(+\hat{z})$$
The fraction of the particles transmitted through the first $SG_z$ device that will survive the third measurement is given by

$$f = \left| \langle \hat{z} | \hat{M}(\hat{z}) \hat{M}(\hat{n}) | +\hat{z} \rangle \right|^2 = \cos^2 \frac{\theta}{2} \sin^2 \frac{\theta}{2} = \frac{1}{4} \sin^2 \theta$$

(b) How must the angle $\theta$ of the $SG_n$ device be oriented so as to maximize the number of particles that are transmitted by the final $SG_z$ device? What fraction of the particles survive the third measurement for this value of $\theta$?

This is maximized by choosing $\theta = \pi/2$ so that $f_{\text{max}} = 1/4$.

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

If there is no third device, then the fraction surviving is

$$f = \left| \langle +\hat{n} | \hat{M}(+\hat{n}) | +\hat{z} \rangle \right|^2 = \left| \langle +\hat{n} | (\cos^2 \frac{\theta}{2} + \cos \frac{\theta}{2} \sin \frac{\theta}{2}) | +\hat{z} \rangle \right|^2$$

$$= \left| \cos^2 \frac{\theta}{2} + \cos \frac{\theta}{2} \sin \frac{\theta}{2} \right|^2 = \cos^4 \frac{\theta}{2} (1 + \sin 2\theta)$$

7.5.10 Orientations

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

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

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

For a general linearly polarized state at angle $\theta$ we have the state vector

$$|\psi\rangle = \cos \theta |h\rangle + \sin \theta |v\rangle$$

For

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

we have

$$\cos \theta = -\frac{1}{2} , \quad \sin \theta = -\frac{\sqrt{3}}{2}$$

or $\theta = 210^\circ = -150^\circ$.

For

$$|\psi_2\rangle = -\frac{1}{2} \left( |h\rangle - \sqrt{3} |v\rangle \right)$$
we have
\[ \cos \theta = -\frac{1}{2}, \quad \sin \theta = \frac{\sqrt{3}}{2} \]
or \( \theta = 330^\circ = -30^\circ \).

For
\[ |\psi_2\rangle = |h\rangle \]
we have
\[ \cos \theta = 1, \quad \sin \theta = 0 \]
or \( \theta = 0^\circ \).

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,
\[ |K'_L\rangle = (1 + \varepsilon) |K^0\rangle - (1 - \varepsilon) |\bar{K}^0\rangle \]
where \( \varepsilon \) is a very small complex number (|\varepsilon| \approx 2 \times 10^{-3}) 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 \( e^{-i\omega_L t -it/2\tau_L} \) (or \( e^{-i\omega_S t -it/2\tau_S} \)) where
\[ h\omega_L = (p^2 c^2 + m^2_L c^4)^{1/2} \quad \text{(or) } h\omega_S = (p^2 c^2 + m^2_S c^4)^{1/2} \]
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 \( |\bar{K}^0\rangle \).

We have
\[ |K'_L\rangle = A \left[ (1 + \varepsilon) |K^0\rangle - (1 - \varepsilon) |\bar{K}^0\rangle \right] \]
where \( A \) is the normalization factor. We then have
\[ \langle K'_L | K'_L \rangle = |A_L|^2 \left[ (1 + \varepsilon^*) \langle K^0 | - (1 - \varepsilon^*) \langle \bar{K}^0 | \right] \left[ (1 + \varepsilon) |K^0\rangle - (1 - \varepsilon) |\bar{K}^0\rangle \right] \]
\[ = 2 |A_L|^2 \left( 1 + |\varepsilon|^2 \right) = 1 \]
or
\[ A_L = \frac{1}{\sqrt{2(1 + |\varepsilon|^2)}} \]

Now we must also have
\[ \langle K'_S | K'_S \rangle = 1, \quad \langle K'_S | K'_L \rangle = 0 \]
We assume that

\[ |K'_L⟩ = [a |K^0⟩ + b |\bar{K}^0⟩] \]

and we get

\[ |a|^2 + |b|^2 = 1, \quad a^* (1 + \varepsilon) - b^* (1 - \varepsilon) = 0 \]

If we choose

\[ a = \frac{1 - \varepsilon^*}{\sqrt{2(1 + |\varepsilon|^2))}}, \quad b = \frac{1 + \varepsilon^*}{\sqrt{2(1 + |\varepsilon|^2)}} \]

then both the conditions are satisfied so that

\[ |K'_L⟩ = \frac{1}{\sqrt{2(1 + |\varepsilon|^2))}} \left[ (1 + \varepsilon) |K^0⟩ - (1 - \varepsilon) |\bar{K}^0⟩ \right] \]
\[ |K'_S⟩ = \frac{1}{\sqrt{2(1 + |\varepsilon|^2))}} \left[ (1 - \varepsilon^*) |K^0⟩ + (1 + \varepsilon^*) |\bar{K}^0⟩ \right] \]

or rewriting in the (|K_L⟩, |K_S⟩) basis we have

\[ |K'_L⟩ = \frac{1}{\sqrt{2(1 + |\varepsilon|^2))}} \left[ (1 + \varepsilon) \frac{1}{\sqrt{2}} (|K_L⟩ + |K_S⟩) - (1 - \varepsilon) \frac{1}{\sqrt{2}} (|K_S⟩ - |K_L⟩) \right] \]
\[ = \frac{1}{\sqrt{1 + |\varepsilon|^2)} (|K_L⟩ + \varepsilon |K_S⟩) \]

\[ |K'_S⟩ = \frac{1}{\sqrt{2(1 + |\varepsilon|^2))}} \left[ (1 - \varepsilon^*) \frac{1}{\sqrt{2}} (|K_L⟩ + |K_S⟩) + (1 + \varepsilon^*) \frac{1}{\sqrt{2}} (|K_S⟩ - |K_L⟩) \right] \]
\[ = \frac{1}{\sqrt{1 + |\varepsilon|^2)} (|K_S⟩ - \varepsilon^* |K_L⟩) \]

and

\[ |K'_L(t)⟩ = \frac{1}{\sqrt{(1 + |\varepsilon|^2)}} \left( e^{-i\omega_L t - t/2\tau_L} |K_L⟩ + \varepsilon e^{-i\omega_{SL} t - t/2\tau_S} |K_S⟩ \right) \]
\[ |K'_S(t)⟩ = \frac{1}{\sqrt{(1 + |\varepsilon|^2)}} \left( e^{-i\omega_S t - t/2\tau_S} |K_S⟩ - \varepsilon^* e^{-i\omega_{SL} t - t/2\tau_L} |K_L⟩ \right) \]

(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 \( \varepsilon \)?

We are interested in the ratio

\[ R = \frac{|(CP = +1 | K'_L(t)⟩|^2}{|(CP = -1 | K'_S(t)⟩|^2} = \frac{|(K_S | K'_L(t)⟩|^2}{|(K_S | K'_S(t)⟩|^2} \]
Notice that if $|K'_{L}\rangle \rightarrow |K_{L}\rangle$, then the probability for it to behave like a $|K_{S}\rangle$ would be zero. This means that if we see any effect (any $CP = +1$ decays), that is, if $\varepsilon \neq 0$, this result implies non-conservation of $CP$.

We get

$$R = \frac{|\langle K_{S} | K'_{L}(t) \rangle|^{2}}{|\langle K_{S} | K'_{S}(t) \rangle|^{2}} = \frac{1}{(1+|\varepsilon|^{2})} \left| \frac{\varepsilon^{2}}{e^{-t/\tau_{L}}} \right| = \frac{|\varepsilon|^{2}}{e^{(1/\tau_{S} - 1/\tau_{L})}}$$

Therefore, measuring this ratio (Fitch/Cronin 1963) gives $|\varepsilon|$.

(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 $\delta$. 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 $\delta$) enable one to determine the phase of $\varepsilon$?

The number of two pion events ($CP = -1$) is proportional to the probability $P_{K'_{L} \rightarrow K_{S}}(t) = |\langle K_{S} | K'_{L}(t) \rangle|^{2}$ so we will calculate that quantity.

We have before the absorber

$$|\psi_{before}\rangle = |K'_{L}\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^{2})}} \left[ (1+\varepsilon) |K_{0}\rangle - (1-\varepsilon) |\bar{K}_{0}\rangle \right]$$

and after the absorber

$$|\psi_{after}\rangle = |\psi(0)\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^{2})}} \left[ (1+\varepsilon) |K_{0}\rangle - e^{-i\delta} (1-\varepsilon) |\bar{K}_{0}\rangle \right]$$

$$= \frac{1}{\sqrt{2(1+|\varepsilon|^{2})}} \left[ (1+\varepsilon) \frac{1}{\sqrt{2}} (|K_{L}\rangle + |K_{S}\rangle) - e^{-i\delta} (1-\varepsilon) \frac{1}{\sqrt{2}} (|K_{S}\rangle - |K_{L}\rangle) \right]$$

$$= \frac{1}{2\sqrt{(1+|\varepsilon|^{2})}} \left[ ((1+\varepsilon) - e^{-i\delta} (1-\varepsilon)) |K_{S}\rangle + ((1+\varepsilon) + e^{-i\delta} (1-\varepsilon)) |K_{L}\rangle \right]$$

so that

$$|K'_{L}(t)\rangle = \frac{1}{2\sqrt{(1+|\varepsilon|^{2})}} \left[ ((1+\varepsilon) - e^{-i\delta} (1-\varepsilon)) e^{-i\omega_{S}t - t/2\tau_{S}} |K_{S}\rangle + ((1+\varepsilon) + e^{-i\delta} (1-\varepsilon)) e^{-i\omega_{L}t - t/2\tau_{L}} |K_{L}\rangle \right]$$

and

$$P_{K'_{L} \rightarrow K_{S}}(t) = |\langle K_{S} | K'_{L}(t) \rangle|^{2} = \frac{1}{4(1+|\varepsilon|^{2})} \left| (1+\varepsilon) - e^{-i\delta} (1-\varepsilon) \right|^{2} e^{-t/\tau_{S}}$$
This is the probability of two pion events as a function of time.

Now
\[ \left| (1 + \varepsilon) - e^{-i\delta} (1 - \varepsilon) \right|^2 = ((1 + \varepsilon^*) - e^{i\delta} (1 - \varepsilon^*)) (1 + \varepsilon) - e^{-i\delta} (1 - \varepsilon) \]
\[ = (1 + \varepsilon^*) (1 + \varepsilon) + (1 - \varepsilon^*) (1 - \varepsilon) - (1 + \varepsilon^*) (1 - \varepsilon) e^{-i\delta} - (1 - \varepsilon^*) (1 + \varepsilon) e^{i\delta} \]
\[ = 1 + \varepsilon^* + \varepsilon + |\varepsilon|^2 + 1 - \varepsilon^* - \varepsilon + |\varepsilon|^2 - \left( 1 + \varepsilon^* - \varepsilon - |\varepsilon|^2 \right) e^{-i\delta} - \left( 1 - \varepsilon^* + \varepsilon - |\varepsilon|^2 \right) e^{i\delta} \]
\[ = 2 + 2 |\varepsilon|^2 - 2 \left( 1 - |\varepsilon|^2 \right) \cos \delta + 2i (\varepsilon^* - \varepsilon) \sin \delta \]
\[ = 2(1 - \cos \delta) + 2 |\varepsilon|^2 (1 + \cos \delta) + 2\text{Im}(\varepsilon) \sin \delta \]
so that
\[ P_{K_L \rightarrow K_S}(t) = \frac{1}{1 + |\varepsilon|^2} \left( 1 - \cos \delta + |\varepsilon|^2 (1 + \cos \delta) + \text{Im}(\varepsilon) \sin \delta \right) e^{-t/\tau_S} \]

Now measuring $R \rightarrow |\varepsilon|$ and then measuring $P_{K_L \rightarrow K_S}(t) \rightarrow \text{Im}(\varepsilon)$. We then have
\[ \text{Re}(\varepsilon) = \sqrt{|\varepsilon|^2 - (\text{Im}(\varepsilon))^2} \rightarrow \text{phase}(\varepsilon) = \varphi = \tan^{-1} \frac{\text{Re}(\varepsilon)}{\text{Im}(\varepsilon)} = \tan^{-1} \frac{\sqrt{|\varepsilon|^2 - (\text{Im}(\varepsilon))^2}}{\text{Im}(\varepsilon)} \]

7.5.12 Quarter-wave plate

A beam of linearly polarized light is incident on a quarter-wave plate (changes relative phase by $90^\circ$) with its direction of polarization oriented at $30^\circ$ 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.

We have for a quarter-wave plate
\[ \hat{Q} = |x\rangle \langle x| + e^{i\pi/2} |y\rangle \langle y| \rightarrow \text{changes relative phase by } \pi/2 \]
The input state is
\[ |in\rangle = \cos 30^\circ |x\rangle + \sin 30^\circ |y\rangle = \frac{\sqrt{3}}{2} |x\rangle + \frac{1}{2} |y\rangle \]
Therefore, after the 1/4-wave plate we have
\[ |out\rangle = \hat{Q} |in\rangle = \frac{\sqrt{3}}{2} |x\rangle + \frac{1}{2} e^{i\pi/2} |y\rangle = \frac{\sqrt{2}}{2} |x\rangle + \frac{i}{2} |y\rangle \]
Then
\[ \langle R | out\rangle = \frac{1}{\sqrt{2}} (\langle x | - i \langle y |) \left( \frac{\sqrt{2}}{2} |x\rangle + \frac{i}{2} |y\rangle \right) = \frac{\sqrt{3} + 1}{2\sqrt{2}} \]
\[ P_R = |\langle R | \text{out} \rangle|^2 \]

\[ BraketL_{out} = \frac{1}{\sqrt{2}} (|x\rangle + i |y\rangle) \left( \frac{\sqrt{2}}{2} |x\rangle + \frac{i}{2} |y\rangle \right) = -\frac{\sqrt{3}}{2} + \frac{1}{2\sqrt{2}} \]

\[ P_L = |\langle L | \text{out} \rangle|^2 \]

Therefore, the rate at which angular momentum is absorbed by the disk is

\[ N\hbar (P_R - P_L) = \frac{\sqrt{3}}{2} N\hbar \]

Thus, the torque is positive, which implies that the disk will rotate CCW as viewed from the positive \( z \)-axis.

### 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 \( \varphi/N \) with the \( y \)-axis. The transmission axis of every other polarizer makes an angle \( \varphi/N \) with respect to the axis of the preceding polarizer. Thus, the transmission axis of the final polarizer makes an angle \( \varphi \) 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?

Photons exiting the last polaroid are in the state \( |y'(\varphi)\rangle \), polarized at angle \( \varphi \) with respect to the \( y \)-axis.

The probability of passing through the first polaroid is

\[ |\langle y'(\varphi/N) | y \rangle|^2 = \cos^2 \frac{\varphi}{N} \]

so that the probability of being transmitted by the entire array is

\[ \left( \cos^2 \frac{\varphi}{N} \right)^N \]

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

For large \( N \), \( \varphi/N \ll \) so that

\[ \cos \frac{\varphi}{N} \approx 1 - \frac{1}{2} \left( \frac{\varphi}{N} \right)^2 \rightarrow \cos^2 \frac{\varphi}{N} \approx 1 - \left( \frac{\varphi}{N} \right)^2 \]

Therefore, the total probability of transmission for large \( N \) is

\[ \left( 1 - \left( \frac{\varphi}{N} \right)^2 \right)^N \approx 1 - N \left( \frac{\varphi}{N} \right)^2 = 1 - \frac{\varphi^2}{N} \lim_{N \to \infty} 1 \]
(c) Consider the special case with the angle 90°. Explain why your result is not in conflict with the fact that \( \langle x | y \rangle = 0 \).

For \( \varphi = 90° \), \( (|y\rangle = |x\rangle) \), the total probability is not equal to \( |\langle x | y \rangle|^2 = 0 \), but rather approaches unity as \( N \to \infty \). The array of polarizers actually makes an infinite series of measurements of the polarization, each of which rotates the state of the exiting photon!!

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

\[
|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = e^{-i\hbar\nu t/\hbar} |\psi(0)\rangle = e^{-i2\pi\nu t/\hbar} |\psi(0)\rangle = e^{-i2\pi x/\lambda} |\psi(0)\rangle
\]

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 and emit photons at the same time. Let the distance between the two sources be \( L \).

\[ \text{Figure 7.2: Interference Setup} \]

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

\[
P(x) = |\langle \psi(t) | \psi(t) \rangle|^2 = |e^{-2\pi i x/\lambda} + e^{-2\pi i (L-x)/\lambda}|^2 |\langle \psi(0) | \psi(0) \rangle|^2
\]

\[
= |e^{-2\pi i x/\lambda} + e^{-2\pi i L/\lambda} e^{2\pi i x/\lambda}|^2
\]

\[
= |e^{2\pi i (x-L)/\lambda} + e^{-2\pi i (x-L/2)/\lambda}|^2
\]

\[
= 4 \cos^2 \left( \frac{2\pi}{\lambda} \left( x - \frac{L}{2} \right) \right)
\]

(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?

The result is showing an interference pattern between the two sources. For light waves it corresponds to constructive and destructive interference.

### 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](image)

We calculate PLD as follows:

\[
PLD = d \sin \theta = d \left[ \frac{y}{\sqrt{L^2 + y^2}} \right] \approx \frac{yd}{L} , \quad y \ll L
\]
Show that the relative probability of detecting a photon at various points along the screen is approximately equal to

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

Using the result of 7.5.14 we have

\[ |\text{screen at } y\rangle = |\psi(y)\rangle = e^{-i2\pi S_1/\lambda} |\psi_0\rangle + e^{-i2\pi S_2/\lambda} |\psi_0\rangle \]

Thus, the probability of detection at \( y \) is

\[ |\langle \psi(y) | \psi(y) \rangle|^2 = |e^{-i2\pi S_1/\lambda} + e^{-i2\pi S_2/\lambda}|^2 \text{ vert } |\psi_0\rangle |\psi_0\rangle|^2 \]

and the relative probability is

\[ P(y) = |e^{-i2\pi S_1/\lambda} + e^{-i2\pi S_2/\lambda}|^2 = |e^{i\pi(S_2-S_1)/\lambda} + e^{-i\pi(S_2-S_1)/\lambda}|^2 \]

or

\[ P(y) = 4 \cos^2 \left( \frac{\pi(S_2 - S_1)}{\lambda} \right) = 4 \cos^2 \left( \frac{\pi y d}{\lambda L} \right) \]

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 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).

![Beam Splitter](image)

Figure 7.4: Beam Splitter

The input-output transformation of the waves incident on 50-50 beam splitters and perfectly reflecting mirrors are shown in the figure below.
(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.

We have

\[ \psi_{1,\text{out}} = \frac{1}{\sqrt{2}} \psi_{\text{in}}, \quad \psi_{2,\text{out}} = \frac{1}{\sqrt{2}} \psi_{\text{in}} \]

since nothing enters part #2. By the Born rule, the probability to find a photon a position 1 or 2 is

\[ P_{1,\text{out}} = \int |\psi_{1,\text{out}}|^2 dx = \frac{1}{2} \int |\psi_{\text{in}}|^2 dx = \frac{1}{2} \]

\[ P_{2,\text{out}} = \int |\psi_{2,\text{out}}|^2 dx = \frac{1}{2} \int |\psi_{\text{in}}|^2 dx = \frac{1}{2} \]

There is a 50-50 chance of either result.

NOTE: The photon is found at one detector or the other, never both. The photon is indivisible. This contrasts with classical waves where half of the intensity goes along one way and half the other; an antenna would also receive energy. We interpret this as the mean value of a large number of photons.

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

The wave function is split at b1, sent along two different paths, and recombined at b2. To find the wavefunctions impinging on D1 and D2 we apply the transformation rules sequentially.

Beam splitter #1:

Propagation a distance $L/2$:

$\rightarrow$ phase $e^{ikL/2}$

Bounce off mirrors:
Another propagation by a distance $L/2$:

$\rightarrow phase \ e^{ikL}$

Beam splitter #2:
where

\[
\psi_{\text{out},1} = \frac{\psi_{\text{in},1} + \psi_{\text{in},2}}{\sqrt{2}} = e^{ikL}\psi_{\text{in}} \\
\psi_{\text{out},2} = \frac{\psi_{\text{in},1} - \psi_{\text{in},2}}{\sqrt{2}} = 0
\]

Therefore,

\[
P_{\text{out},1} = \int dx |\psi_{\text{out},1}|^2 = \int dx |\psi_{\text{in}}|^2 = 1 \\
P_{\text{out},2} = \int dx |\psi_{\text{out},2}|^2 = 0
\]

which implies that there is a 100% chance of detector D1 firing and a 0% chance of detector D2 firing. There is no randomness!!

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

\[
P_{D1} = P(\text{transmission at } b2|\text{green path})P(\text{green path}) + P(\text{reflection at } b2|\text{blue path})P(\text{blue path})
\]

Calculate this and compare to the quantum result. Explain.

The above expression is the probability of the the green path being taken + the probability of the blue path being taken. Now we know that there is a 50-50 probability for the photon to take the blue or green path which implies that

\[
P(\text{blue}) = P(\text{green}) = \frac{1}{2}
\]

Also with the particle incident at b2 along the green path there is a 50% chance of transmission and similarly for reflection of the blue path. This implies that

\[
P(\text{transmission at } b2|\text{green path}) = P(\text{reflection at } b2|\text{blue path}) = \frac{1}{2}
\]

Therefore

\[
P_{D1} = \frac{1}{2} \times \frac{1}{2} + \frac{1}{2} \times \frac{1}{2} = \frac{1}{2}
\]
Thus, classical reasoning implies a 50-50 chance of D1 firing, i.e., it is completely random!!

The quantum case is different because the two paths which lead to detector D1 are indistinguishable and hence the amplitudes interfere, i.e.,

$$\psi_{\text{total}} = \frac{1}{\sqrt{2}} \psi_{\text{in}} e^{ikL} + \frac{1}{\sqrt{2}} \psi_{\text{in}} e^{ikL}$$

so that

$$P_{D1} = \int dx |\psi_{\text{total}}|^2 = \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} = 1$$

where the last two terms are the interference terms. The paths that lead to detector D2 destructively interfere and hence $P_{D2} = 0$.

(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.

We now want constructive interference for the paths that lead to D2 and destructive for D1.

We can achieve this by changing the relative phase of the two paths by moving one of the mirrors so that the path lengths are now different (unbalanced). We have

$$\psi_{1,\text{out}} = \frac{1}{\sqrt{2}} \psi_{\text{in}} e^{ikL+\Delta L} + \frac{1}{\sqrt{2}} \psi_{\text{in}} e^{ikL}$$

$$\psi_{2,\text{out}} = \frac{1}{\sqrt{2}} \psi_{\text{in}} e^{ikL+\Delta L} - \frac{1}{\sqrt{2}} \psi_{\text{in}} e^{ikL}$$

We then have

$$P_{D1} = \int dx |\psi_{1,\text{out}}|^2 = \frac{1}{4} \int dx |\psi_{\text{in}} e^{ikL+\Delta L} + \psi_{\text{in}} e^{ikL}|^2$$

$$= \frac{1}{4} \int dx |\psi_{\text{in}}|^2 |e^{ikL}|^2 |e^{ik\Delta L} + 1|^2$$

$$= \frac{1}{4} (e^{ik\Delta L} + 1)(e^{-ik\Delta L} + 1) = \frac{1 + \cos (k\Delta L)}{2}$$

$$= \cos^2 \left( \frac{k \Delta L}{2} \right)$$

Similarly,

$$P_{D2} = \frac{1 - \cos (k\Delta L)}{2} = \sin^2 \left( \frac{k \Delta L}{2} \right)$$
Thus, to achieve $P_{D1} = 0$, $P_{D2} = 1$, we choose $k\Delta L = m\pi$, $m$ odd, which implies that $\Delta L = m\lambda/2$. Generally the probability if detection in D1 and D2 as a function of $\Delta L$ look like

These are the interference fringes associated with this interferometer.

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).

![Mach-Zender Setups](image)

A transparent piece of glass which imparts a phase shift (PS) $\phi$ 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 $\phi$ for each device. Explain your answer.

In interferometer (i) there are two paths (reflection and transmission at second beam splitter) which can lead to detection at D. These probability amplitudes interfere as in 7.5.16(d).

In phase $\rightarrow$ constructive interference ($\phi = 0, 2\pi, 4\pi, ...$)

Out of phase $\rightarrow$ destructive interference ($\phi = 0, \pi, 3\pi, 5\pi, ...$)
As in 7.5.16(d) a plot of $P_D$ oscillates between those values.

Without the final beam splitter, there is only one path that leads to D (the top path). Therefore, there is no interference which implies that there is always a 50% chance of hitting the detector. A plot of $P_D$ is constant at $1/2$. 
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 $\lambda$ 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](image)

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

We have two regions to consider:

**Region I:** $0 \leq x \leq L/2$ The solution is

$$\psi_I(x) = A_1 \sin kx$$
which already incorporates the boundary condition \( \psi_I(x = 0) = 0 \).

**Region II**: \( L/2 \leq x \leq L \) The solution is
\[
\psi_{II}(x) = A_2 \sin k(x - L)
\]
which already incorporates the boundary condition \( \psi_{II}(x = L) = 0 \).

At \( x = L/2 \), we have
\[
\psi_I(x = L/2) = \psi_{II}(x = L/2) \rightarrow A_1 = A_2
\]
The first derivative is discontinuous at \( x = L/2 \) and we have
\[
\psi'_{II}(x = L/2) - \psi'_I(x = L/2) = \frac{2m\lambda}{\hbar^2} \psi_I(x = L/2)
\]
or
\[
-A_1 k \cos \frac{kL}{2} - A_1 k \cos \frac{kL}{2} = \frac{2m\lambda}{\hbar^2} \sin \frac{kL}{2} \rightarrow \tan \frac{kL}{2} = -\frac{\hbar^2}{m\lambda} k
\]
Therefore, we have a transcendental equation for
\[
k \rightarrow E = \frac{\hbar^2 k^2}{2m}
\]

**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
\[
\psi(x, t = 0) = \sqrt{\frac{8}{5a}} \left( 1 + \cos \left( \frac{\pi x}{a} \right) \right) \sin \left( \frac{\pi x}{a} \right)
\]
For an infinite square well we have
\[
\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n = 1, 2, 3, \ldots.
\]
And any arbitrary wave function can be expanded in this basis, that is,
\[
\psi(x, t) = \sum_n A_n e^{-iE_n t/\hbar} \psi_n(x)
\]
We have
\[
\psi(x, t = 0) = \sqrt{\frac{8}{5a}} \left( 1 + \cos \left( \frac{\pi x}{a} \right) \right) \sin \left( \frac{\pi x}{a} \right)
\]
This can be written
\[
\psi(x, t = 0) = \sqrt{\frac{8}{5a}} \left( 1 + \cos \left( \frac{\pi x}{a} \right) \right) \sin \left( \frac{\pi x}{a} \right)
\]
\[
= \sqrt{\frac{8}{5a}} \sin \left( \frac{\pi x}{a} \right) + \sqrt{\frac{2}{5a}} \sin \left( \frac{2\pi x}{a} \right)
\]
\[
= \sqrt{\frac{4}{5}} \psi_1(x) + \sqrt{\frac{1}{5}} \psi_2(x)
\]

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which is a sum of eigenfunctions.

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

At time $t$ we then have

$$
\psi(x, t_0) = \sqrt{\frac{4}{5}} e^{-iE_1 t_0/\hbar} \psi_1(x) + \sqrt{\frac{1}{5}} e^{-iE_2 t_0/\hbar} \psi_2(x)
$$

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

The average energy does not change so that

$$
\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle = \sum_n E_n |A_n|^2 = E_1 |A_1|^2 + E_2 |A_2|^2 = \frac{4}{5} E_1 + \frac{1}{5} E_2 = \frac{4\pi^2 \hbar^2}{5ma^2}
$$

(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 $t = t_0$?

The probability that the particle is in the region $0 \leq x \leq a/2$ at $t = t_0$ is

$$
P(0 \leq x \leq a/2; t_0) = \int_0^{a/2} |\psi(x, t_0)|^2 dx
$$

where

$$
|\psi(x, t_0)|^2 = e^{-iE_1 t_0/\hbar} \left| e^{-iE_1 t_0/\hbar} \sqrt{\frac{8}{5a}} \sin \left( \frac{\pi x}{a} \right) \left( 1 + \cos \left( \frac{\pi x}{a} \right) e^{-i(E_2 - E_1) t_0/\hbar} \right) \right|^2
$$

$$
= \frac{8}{5a} \sin^2 \left( \frac{\pi x}{a} \right) \left( 1 + \cos^2 \left( \frac{\pi x}{a} \right) + 2 \cos \left( \frac{\pi x}{a} \right) \cos \frac{3\pi^2 \hbar^2}{2ma^2 t_0} \right) + 2 \cos \left( \frac{\pi x}{a} \right) \cos \frac{3\pi^2 \hbar^2}{2ma^2 t_0}
$$

so that

$$
P(0 \leq x \leq a/2; t_0) = \frac{1}{2} + \frac{16}{15\pi} \cos \frac{3\pi^2 \hbar^2}{2ma^2 t_0}
$$

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,

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

(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.

Let us define
\[
\kappa^2 = \frac{2m|E|}{\hbar^2}, \quad q^2 = \frac{2m(|E| + V_0)}{\hbar^2}, \quad \beta^2 = \frac{2mV_0}{\hbar^2}
\]

The Schrodinger equation is
\[
\psi'' = \kappa^2 \psi \quad |x| > a \\
\psi'' = q^2 \psi \quad |x| < a
\]

The discontinuity at the origin gives
\[
\psi'(0+) - \psi'(0-) = -g^2 \psi(0)
\]

Odd parity solutions do not see the attractive delta function (they must be zero at the origin) and thus cannot exist for \( E < 0 \). Even parity solutions of the above equations have the form
\[
\psi(x) = \begin{cases} 
A e^{-\kappa|x|} & |x| > a \\
Be^{q|x|} + Ce^{-q|x|} & |x| < a
\end{cases}
\]

Continuity at \( x = a \) and \( x = 0 \) leads to the condition (eigenvalue equation)
\[
e^{2qa} \frac{1 - g^2/2q}{1 + g^2/2q} = \frac{q - \kappa}{q + \kappa}
\]

In the case of vanishing \( V_0 \), we recover the equation
\[
E_0 = -\frac{\hbar^2}{2m} \left( \frac{g^2}{2} \right)^2
\]
appropiate to a delta function well.

Since the RHS of the eigenvalue equation is always positive, we necessarily have
\[
1 - g^2/2q > 0 \Rightarrow \frac{2m}{\hbar^2} (-E + V_0) \geq \frac{g^4}{4}
\]
or
\[
E \leq V_0 - \frac{\hbar^2}{2m} \left( \frac{g^2}{2} \right)^2 = V + E_0
\]

One can see graphically that the above eigenvalue equation has only one solution, by defining
\[
\xi = qa, \quad \lambda = \frac{g^2 a}{2}, \quad b = \beta a
\]
Then, we have

\[ e^{2\xi} \left( \frac{\xi - \lambda}{\xi + \lambda} \right) = \frac{\xi - \sqrt{\xi^2 - b^2}}{\xi + \sqrt{\xi^2 - b^2}} \]

The solution exists provided that \( \lambda \geq b \). In the limiting case, \( \lambda = b \), or, equivalently,

\[ \beta^2 = \frac{2mV_0}{\hbar^2} = \frac{g^4}{4} \]

we get a vanishing ground state 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?

The wave function will be of the form

\[ \psi(x) = \begin{cases} e^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ikx} & x > 0 \end{cases} \]

with

\[ k = \sqrt{\frac{2mE}{\hbar}} \quad \text{and} \quad q = \sqrt{\frac{2m(E - V)}{\hbar}} \]

Continuity of the wave function at \( x = 0 \) gives

\[ 1 + B = C \]

Integrating the Schrödinger equation over the infinitesimal interval around the origin gives

\[ -\frac{\hbar^2}{2m} (\psi'(0^+) - \psi'(0^-)) = \frac{\hbar^2 g}{2m} \psi(0) \]

\[ 1 - B = -\frac{i}{k} (g + iq)C \]

From the two relationships between \( B \) and \( C \) we obtain

\[ C = \left( \frac{1 + q/k + ig/k}{1 - q/k - ig/k} \right)^2 \]

\[ B = \left( \frac{1 - q/k - ig/k}{1 + q/k + ig/k} \right)^2 \]

The reflection coefficient is

\[ \mathcal{R} = \left| \frac{j_x}{j_t} \right|^2 = \frac{(\hbar k/m) |B|^2}{\hbar k/m} = \left| \frac{1 - q/k + ig/k}{1 + q/k - ig/k} \right|^2 = \frac{(1 - q/k)^2 + g^2/k^2}{(1 + q/k)^2 + g^2/k^2} \]

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In the high energy limit we have
\[ \mathcal{R} = \frac{g \hbar^2}{8 m E} \]

For the pure step barrier we have (in the same limit)
\[ \mathcal{R} = \frac{V^2}{8 E^2} \]

which drops off faster with energy.

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

In order to study the case of negative energy, \( E < 0 \), it is convenient to introduce the notation
\[ \kappa_- = \sqrt{\frac{2m |E|}{\hbar^2}}, \quad \kappa_+ = \sqrt{\frac{2m(V + |E|)}{\hbar^2}} \]

Then we can write the bound-state wave function as
\[ \psi(x) = \begin{cases} A e^{\kappa_- x} & x < 0 \\ A e^{-\kappa_+ x} & x > 0 \end{cases} \]

The discontinuity at the origin implies that
\[ -\frac{\hbar^2}{2m} (-A \kappa_+ - A \kappa_-) = \frac{\hbar^2 g}{2m} A \]

This then gives
\[ E = -\frac{m}{2\hbar^2 g^2} \left( \frac{\hbar^2 g^2}{2m} - V \right)^2 \]
and
\[ \kappa^2 = \frac{m^2}{\hbar^4 g^2} \left( \frac{\hbar^2 g^2}{2m} \pm V \right)^2 \]
and
\[ A = \sqrt{\frac{2 \kappa_+ \kappa_-}{g}} \]

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.

For \( x > -d \), the Schrödinger equation is

\[
\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E + V_0 \delta(x)) \psi = 0
\]

We let

\[
k = \sqrt{-\frac{2mE}{\hbar^2}}
\]

where \( E < 0 \). In the region \( -d < x < 0 \), the solution is

\[
\psi_1(x) = ae^{kx} + be^{-kx}
\]

In the region \( x > 0 \), the solution is

\[
\psi_2(x) = e^{-kx}
\]

At \( x = 0 \), the wave function is continuous so that

\[
\psi_1(0) = a + b = \psi_2(0) = 1
\]

At \( x = 0 \), the first derivative of the wave function is discontinuous since integrating the Schrödinger equation across the discontinuity we find

\[
\lim_{\varepsilon \to 0} \left[ \varepsilon \int_{-\varepsilon}^{\varepsilon} \frac{d^2 \psi}{dx^2} dx + \frac{2m}{\hbar^2} \int_{-\varepsilon}^{\varepsilon} E \psi(x) dx + \frac{2m}{\hbar^2} \int_{-\varepsilon}^{\varepsilon} V_0 \delta(x) \psi(x) dx \right] = 0
\]

\[
0 = \Delta \left( \frac{d\psi}{dx} \right) + \frac{2mV_0}{\hbar^2} \psi(0) \rightarrow \psi_2'(0) - \psi_1'(0) = -\frac{2mV_0}{\hbar^2} \psi_2(0)
\]

\[
-k - k(a - b) = -\frac{2mV_0}{\hbar^2}
\]
At \( x = -d \), we have an infinite well, so that \( \psi_1(-d) = 0 \) or

\[
\begin{align*}
a + b &= 1 \\
-k - k(a - b) &= -\frac{2mV_0}{\hbar^2} \\
ace^{-kd} + be^{kd} &= 0
\end{align*}
\]

with solutions

\[
a = -\frac{e^{2kd}}{1 - e^{2kd}}, \quad b = \frac{1}{1 - e^{2kd}}, \quad k = \frac{mV_0}{\hbar^2} \left(1 - e^{-2kd}\right)
\]

(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.

Now the wall is far away from the particle if \( kd \gg 1 \). This says that as a first approximation we would have

\[
k = \frac{mV_0}{\hbar^2} \left(1 - e^{-2kd}\right) \approx \frac{mV_0}{\hbar^2}
\]

which is just the bound state energy from a single delta-function (isolated) well, that is,

\[
E_\delta = -\frac{\hbar^2 k^2}{2m} = -\frac{1}{2} \frac{mV_0^2}{\hbar^2}
\]

To determine the effect of the wall, we must make a better approximation. We do this by calling

\[
k^{(0)} = \frac{mV_0}{\hbar^2} = 0^{th} \text{- order result}
\]

and then obtaining the 1st-order result by inserting the 0th-order result, that is,

\[
k^{(1)} = \frac{mV_0}{\hbar^2} \left(1 - e^{-2k^{(0)}d}\right) = \frac{mV_0}{\hbar^2} \left(1 - e^{-2\frac{mV_0}{\hbar^2}d}\right)
\]

This gives a bound state energy of

\[
E = -\frac{\hbar^2 k^{(1)2}}{2m} \approx -\frac{\hbar^2}{2m} \left(\frac{mV_0}{\hbar^2}\right)^2 \left(1 - e^{-2\frac{mV_0}{\hbar^2}d}\right)^2
\]

\[
\approx -\frac{mV_0^2}{2\hbar^2} \left(1 - 2e^{-2\frac{mV_0}{\hbar^2}d}\right)
\]

\[
= -\frac{mV_0^2}{2\hbar^2} + \frac{mV_0^2}{\hbar^2} e^{-2\frac{mV_0}{\hbar^2}d}
\]

Therefore, the modification of the energy caused by the wall is

\[
\Delta E = \frac{mV_0^2}{\hbar^2} e^{-2\frac{mV_0}{\hbar^2}d}
\]
Now we have assumed that

\[ \frac{2mV_0 d}{\hbar^2} = 2k(0)d \approx 2kd < < 1 \rightarrow d \approx \frac{1}{k} \approx \frac{1}{k(0)} = \frac{\hbar^2}{mV_0} \]

which is the definition of far away.

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

To find the condition (exact) on \( V_0 \) and \( d \) for the existence of at least one bound state we must look at the exact equation

\[ k = \frac{mV_0}{\hbar^2} (1 - e^{-2kd}) \]

It is always a good idea to plot the functions on either side of the equal sign in a transcendental equation in order to help us understand what is going on. In this case we have

![Figure 8.3: Staircase Function](image)

The condition for the existence of a solution is clear from the graph, that is, the slope of curve #2 (the curve) at the origin must be greater than the slope of curve #1 (the straight line).

Now

\[ \left. \frac{dy_1}{dk} \right|_{k=0} = 1 \quad \text{and} \quad \left. \frac{dy_2}{dk} \right|_{k=0} = \frac{2mV_0 d_0}{\hbar^2} \]
Therefore, if
\[ V_0 d > \frac{\hbar^2}{2m} \]
then there exists 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 \( \psi(x, t) \).

The eigenfunctions and eigenvalues of \( \hat{H} \) for this system are
\[ \psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n = 1, 2, 3, \ldots \]

We then have
\[ \psi(x, t) = \sum_{n=1}^{\infty} a_n \psi_n(x) e^{-i E_n t / \hbar} \]

We evaluate the \( a_n \) coefficients using the initial wavefunction
\[ a_k = \int_0^{a/2} \psi(x, 0) \psi_k(x) dx = \frac{2}{a} \int_0^{a/2} \frac{\sin k\pi x}{a} dx = \frac{2}{k\pi} \left( 1 - \cos \frac{k\pi}{2} \right) \]

Therefore,
\[ \psi(x, t) = \frac{2}{\pi} \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} \frac{1}{n} \left( 1 - \cos \frac{n\pi}{2} \right) \sin \frac{n\pi x}{a} e^{-i \frac{n^2 \pi^2 \hbar^2}{2ma^2} t} \]

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

The probability of being in the \( n \)th eigenstate is
\[ P_n = |a_n|^2 = \frac{4}{n^2 \pi^2} \left( 1 - \cos \frac{n\pi}{2} \right)^2 \]
(c) Derive an expression for average value of particle energy. What is the physical meaning of your result?

We have

\[ \langle E \rangle = \langle \psi | \hat{H} | \psi \rangle = \sum_n E_n P_n = \sum_n E_n |a_n|^2 = \frac{2\hbar^2}{ma^2} \sum_n \left( 1 - \cos \frac{n\pi}{2} \right)^2 \]

which does not converge! It takes an infinite amount of energy to form the initial wavefunction because of the sharp edges!

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.

The corresponding 1D Schrödinger equation is

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} - \frac{e^2}{4x} \psi = E \psi = -|E| \psi \]

since \(E < 0\) for a bound state.

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

For \(x \to \infty\) this equation becomes

\[ \frac{d^2 \psi}{dx^2} - \alpha^2 \psi = 0 \quad , \quad \frac{\hbar^2 \alpha^2}{2m} = |E| \]

which has the solution

\[ \psi(x \to \infty) = e^{-\alpha x} \]

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

The boundary condition at \(x = 0\) is \(\psi(0) = 0\).

(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.

We try the solution

\[ \psi(x) = f(x)e^{-\alpha x} \]
which satisfies all boundary conditions if \( f(0) = 0 \) and \( \lim_{x \to \infty} f(x) e^{-\alpha x} \to 0 \). Substituting into the Schrödinger equation we get

\[
\left( f''(x) - 2\alpha f'(x) + \frac{me^2}{2\hbar^2} f(x) \right) e^{-\alpha x} = 0 \to f''(x) - 2\alpha f'(x) + \frac{me^2}{2\hbar^2} f(x) = 0
\]

The solution to this equation is unique so that we only need to guess an expression for \( f(x) \) that satisfies the equation and the boundary conditions. We find

\[
f(x) = x \text{ with } \alpha = \frac{me^2}{4\hbar^2} = \frac{1}{4a_0}
\]

The full solution is then

\[
\psi(x) = Axe^{-\alpha x}
\]

where \( A \) is the normalization constant.

This is the solution for the ground state since it has zeroes only at the boundaries \((x = 0 \text{ and } x \to \infty)\). We find \( A \) by

\[
1 = A^2 \int_0^\infty |\psi(x)|^2 dx = A^2 \int_0^\infty x^2 e^{-2\alpha x} dx = A^2 \frac{\alpha^2}{8\alpha^3} \int_0^\infty y^2 e^{-y} dy = A^2 \frac{\alpha^2}{8\alpha^3} \Gamma(3) = \frac{A^2}{4\alpha^3} \to A = 2\alpha^{3/2}
\]

(d) Find the ground state energy.

\[
E_0 = -\frac{\hbar^2 \alpha^2}{2m} = -\frac{me^4}{32\hbar^2} = -\frac{e^2}{8a_0} = \frac{1}{4} E_{\text{ground-state}}
\]

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

We then have

\[
\langle \psi | \hat{x} | \psi \rangle = \int_0^\infty \int_0^\infty \langle \psi | x' \rangle \langle x' | \hat{x} | x \rangle \langle x | \psi \rangle dx dx' = \int_0^\infty \int_0^\infty \langle \psi | x' \rangle x \delta(x - x') \langle x | \psi \rangle dx dx' = \int_0^\infty \langle \psi | x \rangle \langle x | \psi \rangle dx = \int_0^\infty |\psi(x)|^2 dx = A^2 \int_0^\infty x^3 e^{-2 \alpha x} dx
\]

\[
= \frac{4\alpha^3}{(2\alpha)^4} \Gamma(4) = \frac{3}{2\alpha} = 6a_0
\]

8.15.8 Using the commutator

Using the coordinate-momentum commutation relation prove that

\[
\sum_n (E_n - E_0) \langle E_n | \hat{x} | E_0 \rangle = \text{constant}
\]
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

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

Since

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

we have

$$[\hat{H}, \hat{x}] = \frac{1}{2m} [\hat{p}^2, \hat{x}] = -\frac{i\hbar}{m}$$

and so

$$[[\hat{H}, \hat{x}], \hat{x}] = -\frac{i\hbar}{m} [\hat{p}, \hat{x}] = -\frac{\hbar^2}{m}$$

Therefore,

$$\langle E_m | [[\hat{H}, \hat{x}], \hat{x}] | E_m \rangle = -\frac{\hbar^2}{m}$$

On the other hand, we also have (using $\hat{H} | E_m \rangle = E_m | E_m \rangle$)

$$\langle E_m | [[\hat{H}, \hat{x}], \hat{x}] | E_m \rangle = \langle E_m | (\hat{H}\hat{x}^2 - 2\hat{x}\hat{H}\hat{x} - \hat{x}^2\hat{H}) | E_m \rangle = 2E_m \langle E_m | \hat{x}^2 | E_m \rangle - 2 \langle E_m | \hat{x}\hat{H}\hat{x} | E_m \rangle$$

and

$$\langle E_m | \hat{x}^2 | E_m \rangle = \sum_n \langle E_m | \hat{x} | E_n \rangle \langle E_n | \hat{x} | E_m \rangle = \sum_n |\langle E_m | \hat{x} | E_n \rangle|^2$$

$$\langle E_m | \hat{x}\hat{H}\hat{x} | E_m \rangle = \sum_n \langle E_m | \hat{x}\hat{H} | E_n \rangle \langle E_n | \hat{x} | E_m \rangle = \sum_n E_n \langle E_m | \hat{x} | E_n \rangle \langle E_n | \hat{x} | E_m \rangle = \sum_n \sum_n \langle E_m | \hat{x} | E_n \rangle \langle E_n | \hat{x} | E_m \rangle$$

Therefore,

$$-\frac{\hbar^2}{m} = \langle E_m | [[\hat{H}, \hat{x}], \hat{x}] | E_m \rangle = 2E_m \langle E_m | \hat{x}^2 | E_m \rangle - 2 \langle E_m | \hat{x}\hat{H}\hat{x} | E_m \rangle = 2E_m \sum_n |\langle E_m | \hat{x} | E_n \rangle|^2 - 2 \sum_n E_n |\langle E_m | \hat{x} | E_n \rangle|^2$$

Setting $m = 0$ we get

$$-\frac{\hbar^2}{m} = 2E_0 \sum_n |\langle E_0 | \hat{x} | E_n \rangle|^2 - 2 \sum_n E_n |\langle E_0 | \hat{x} | E_n \rangle|^2$$

or

$$\sum_n (E_n - E_0) |\langle E_0 | \hat{x} | E_n \rangle|^2 = \frac{\hbar^2}{2m}$$

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8.15.9 Matrix Elements for Harmonic Oscillator

Compute the following matrix elements

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

We have

\[ \hat{x} = x_0 (\hat{a} + \hat{a}^+) \], \quad x_0 = \sqrt{\frac{k}{2m\omega}} \]

\[ \hat{a} | n \rangle = \sqrt{n} | n-1 \rangle, \quad \hat{a}^+ | n \rangle = \sqrt{n+1} | n+1 \rangle \]

We then have

\[ \langle n' | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\langle n' | \hat{a} | n \rangle + \langle n' | \hat{a}^+ | n \rangle) = \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}) \]

From this result we get

\[ \langle n' | \hat{x}^2 | n \rangle = \sum_m \langle n' | \hat{x} | m \rangle \langle m | \hat{x} | n \rangle \]

\[ = \frac{\hbar}{2m\omega} \sum_m \left( \sqrt{m}\delta_{m',m-1} + \sqrt{m+1}\delta_{m',m+1} \right) \left( \sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1} \right) \]

\[ = \frac{\hbar}{2m\omega} \sum_m \left( \sqrt{m(m-1)}\delta_{m',m-2} + \sqrt{(m+1)(m+2)}\delta_{m',m+2} + (2m+1)\delta_{m',m} \right) \]

\[ \times \left( \sqrt{n(n-1)}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1} \right) \]

\[ = \frac{\hbar}{2m\omega} \sum_m \left( \sqrt{m(m-1)}\delta_{m',m-2} + \sqrt{(m+1)(m+2)}\delta_{m',m+2} + (2m+1)\delta_{m',m} \right) \]

\[ \times \left( \sqrt{n(n-1)}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1} \right) \]

\[ \langle n' | \hat{x}^3 | n \rangle = \sum_m \langle n' | \hat{x}^2 | m \rangle \langle m | \hat{x} | n \rangle \]

\[ = \frac{\hbar}{2m\omega} \sum_m \left( \sqrt{n(n-1)}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1} \right) \]

\[ \times \left( \sqrt{m(m-1)}\delta_{m',m-2} + \sqrt{(m+1)(m+2)}\delta_{m',m+2} + (2m+1)\delta_{m',m} \right) \]

\[ \times \left( \sqrt{n(n-1)}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1} \right) \]

\[ = \frac{\hbar}{2m\omega} \sqrt{m\omega_0} (\hat{a} - \hat{a}^+) \]

and thus

\[ \langle n' | \hat{p} | n \rangle = -i \frac{\hbar\omega_0}{2} (\langle n' | \hat{a} | n \rangle - \langle n' | \hat{a}^+ | n \rangle) \]

\[ = -i \frac{\hbar\omega_0}{2} (\sqrt{n}\delta_{n',n-1} - \sqrt{n+1}\delta_{n',n+1}) \]

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so that

\[ \langle n' | \hat{x} \hat{p} | n \rangle = \sum \langle n' | \hat{x} | m \rangle \langle m | p | n \rangle = -\frac{i\hbar}{2} \sum_{m} \left( \sqrt{m} \delta_{n',m-1} + \sqrt{m+1} \delta_{n',m+1} \right) \left( \sqrt{n} \delta_{m,n-1} - \sqrt{n+1} \delta_{m,n+1} \right) \]

\[ = -\frac{i\hbar}{2} \left( \sqrt{n(n-1)} \delta_{n',n-2} - \sqrt{(n+1)(n+2)} \delta_{n',n+2} - 1 \right) \delta_{n',n} \]

**8.15.10 A matrix element**

Show for the one dimensional simple harmonic oscillator

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

where \( \hat{z} \) is the position operator.

We want to evaluate

\[ \langle 0 | e^{ik\hat{z}} | 0 \rangle = \sum_{n=0}^{\infty} \frac{(ik)^n}{n!} \langle 0 | \hat{x}^n | 0 \rangle \]

Now

\[ \langle 0 | \hat{x}^0 | 0 \rangle = \langle 0 | 0 \rangle = 1 \]

\[ \langle 0 | \hat{x}^2 | 0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle 0 | (\hat{a} + \hat{a}^+) | 0 \rangle = 0 \rightarrow \langle 0 | \hat{x}^n | 0 \rangle = 0 \quad n \text{ odd} \]

\[ \langle 0 | \hat{x}^4 | 0 \rangle = \frac{\hbar}{2m\omega} \langle 0 | (\hat{a} \hat{a}^+ + \hat{a}^+ \hat{a}) | 0 \rangle = 3 \left( \frac{\hbar}{2m\omega} \right)^2 \]

\[ \langle 0 | \hat{x}^6 | 0 \rangle = 15 \left( \frac{\hbar}{2m\omega} \right)^3 \quad \langle 0 | \hat{x}^8 | 0 \rangle = 105 \left( \frac{\hbar}{2m\omega} \right)^4 \]

\[ \langle 0 | \hat{x}^{2n} | 0 \rangle = \left( \prod_{j \leq 2n, j \text{ odd}} j \right) \left( \frac{\hbar}{2m\omega} \right)^n \]

Therefore

\[ \langle 0 | e^{ik\hat{z}} | 0 \rangle = \sum_{n=0}^{\infty} \frac{(ik)^n}{n!} \langle 0 | \hat{x}^n | 0 \rangle = 1 - \frac{k^2}{2!} \langle 0 | \hat{x}^2 | 0 \rangle + \frac{k^4}{4!} \langle 0 | \hat{x}^4 | 0 \rangle - \frac{k^6}{6!} \langle 0 | \hat{x}^6 | 0 \rangle + ... \]

\[ = 1 - \frac{k^2}{2!} \frac{\hbar}{2m\omega} + \frac{k^4}{4!} 3 \left( \frac{\hbar}{2m\omega} \right)^2 - \frac{k^6}{6!} 15 \left( \frac{\hbar}{2m\omega} \right)^3 + ... \]

\[ = 1 - \frac{1}{11!} \frac{k^2}{2} \langle 0 | \hat{x}^2 | 0 \rangle + \frac{1}{2!} \left( \frac{k^2}{2} \langle 0 | \hat{x}^2 | 0 \rangle \right)^2 - \frac{1}{3!} \left( \frac{k^2}{2} \langle 0 | \hat{x}^2 | 0 \rangle \right)^3 + .... \]

Alternatively, we can use the result

\[ e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2} [\hat{A}, \hat{B}]} \]
to get
\[ \langle 0 | e^{i k \hat{x}} | 0 \rangle = e^{\frac{\hbar k^2}{4m \omega}} \langle 0 | e^{i k \sqrt{\frac{\hbar}{2m \omega}} (\hat{a} + \hat{a}^\dagger)} | 0 \rangle = e^{\frac{\hbar k^2}{4m \omega}} e^{i k \sqrt{\frac{\hbar}{2m \omega}} \hat{a}^\dagger} \langle 0 | e^{i k \sqrt{\frac{\hbar}{2m \omega}} \hat{a}} | 0 \rangle \]

Now expanding the exponential operators we have
\[
\langle 0 | e^{i k \hat{x}} | 0 \rangle = e^{\frac{\hbar k^2}{4m \omega}} | 0 \rangle \left( 1 + i k \sqrt{\frac{\hbar}{2m \omega}} \hat{a} + \frac{1}{2} \left( i k \sqrt{\frac{\hbar}{2m \omega}} \right)^2 \hat{a}^2 + ... \right) \times \left( 1 + i k \sqrt{\frac{\hbar}{2m \omega}} \hat{a}^\dagger + \frac{1}{2} \left( i k \sqrt{\frac{\hbar}{2m \omega}} \right)^2 \hat{a}^\dagger + ... \right)
\]
\[= e^{\frac{\hbar k^2}{4m \omega}} \left( 1 - \frac{k^2 \hbar}{2m \omega} + \frac{k^4 \hbar^2}{8m^2 \omega^2} - ... \right) = e^{\frac{\hbar k^2}{4m \omega}} e^{-\frac{\hbar k^2}{2m \omega}} = e^{-\frac{\hbar k^2}{4m \omega}} \]

Since
\[ \langle 0 | \hat{x}^2 | 0 \rangle = \frac{\hbar}{2m \omega} \]
we have
\[ \langle 0 | e^{i k \hat{x}} | 0 \rangle = e^{-\frac{k^2 \hbar}{4m \omega}} \langle 0 | \hat{x}^2 | 0 \rangle \]
as above.

**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.

We first need to evaluate \( \hat{x}(t) \) in the Heisenberg picture. Since
\[ \hat{x}(t) = \sqrt{\frac{\hbar}{2m \omega}} (\hat{a}(t) + \hat{a}^\dagger(t)) \]
we just need to figure out \( \hat{a}(t) \). Now
\[ \hat{a}(t) = e^{i \hat{H}t/\hbar} \hat{a} e^{-i \hat{H}t/\hbar} \]
where \( \hat{H} = \hbar \omega (\hat{a}^\dagger \hat{a} + 1/2) \). Using the result of an earlier problem we have
\[ \hat{a}(t) = e^{i \hat{H}t/\hbar} \hat{a} e^{-i \hat{H}t/\hbar} = \hat{a} + \frac{i \hbar}{\hbar} \left[ \hat{H}, \hat{a} \right] + \frac{1}{2} \left( \frac{i \hbar}{\hbar} \right)^2 \left[ \hat{H}, \left[ \hat{H}, \hat{a} \right] \right] + ... \]

Now
\[ \left[ \hat{H}, \hat{a} \right] = \hbar \omega \left[ \hat{a}^\dagger \hat{a}, \hat{a} \right] = \hbar \omega (\hat{a}^\dagger \hat{a} \hat{a}^\dagger - \hat{a}^\dagger \hat{a}^\dagger \hat{a}) = -\hbar \omega \hat{a} \]

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so that
\[ \hat{a}(t) = \hat{a} - i\omega \hat{a} + \frac{1}{2} (i\omega)^2 \hat{a} - \frac{1}{6} (i\omega)^3 \hat{a} + \ldots = e^{-i\omega t} \hat{a} \]
and similarly,
\[ \hat{a}^+(t) = e^{i\omega t} \hat{a}^+ \]
so that
\[ \hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}} (e^{-i\omega t} \hat{a} + e^{i\omega t} \hat{a}^+) \]
In the same way we find that
\[ \hat{p}(t) = i\sqrt{\frac{\hbar m\omega}{2}} (e^{i\omega t} \hat{a}^+ - e^{-i\omega t} \hat{a}) \]
Finally, writing \( \hat{x}(0) = \hat{x} \) and \( \hat{p}(0) = \hat{p} \) some algebra shows that
\[ \hat{x}(t) = \hat{x}(0) \cos \omega t + \frac{\hat{p}(0)}{m\omega} \sin \omega t \]
Now we can evaluate the correlation function
\[ C(t) = \langle 0 \mid \hat{x}(t) \hat{x}(0) \mid 0 \rangle \]
\[ = \langle 0 \mid \sqrt{\frac{\hbar}{2m\omega}} (e^{-i\omega t} \hat{a} + e^{i\omega t} \hat{a}^+) \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+) \mid 0 \rangle \]
\[ = \frac{\hbar}{2m\omega} \langle 0 \mid e^{-i\omega t} (0 \hat{a} \hat{a}^+ \mid 0) \rangle = \frac{\hbar}{2m\omega} e^{-i\omega t} \]
All other terms are zero since
\[ \langle 0 \mid \hat{a} \hat{a} \mid 0 \rangle = 0 = \langle 0 \mid \hat{a}^+ \hat{a} \mid 0 \rangle = \langle 0 \mid \hat{a}^+ \hat{a}^+ \mid 0 \rangle \]

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?

We have
\[ P(0) = |\langle 0 \mid \psi \rangle|^2 = \left| \langle 0 \mid e^{-ip_0 x/\hbar} |0\rangle \right|^2 \]
Now use the identity
\[ e^{A+B} = e^A e^B e^{-[A,B]/2} \]
which holds when $[A, B]$ is a c-number, with the operator
\[
x = \sqrt{\frac{\hbar}{2m\omega}} (a^+ + a)
\]
where $[a, a^+] = 1$. Thus,
\[
e^{-ip_0 z/\hbar} = e^{-ip_0 \sqrt{\frac{\hbar}{2m\omega}} (a^+ + a)/\hbar} = e^{-ip_0 \sqrt{\frac{\hbar}{2m\omega}} a^+/\hbar} e^{-ip_0 \sqrt{2m\omega}/4m\hbar}
\]
Therefore, we have
\[
P(0) = e^{-p_0^2/2m\hbar} \left| 0 \right> e^{-ip_0 \sqrt{\frac{\hbar}{2m\omega}} a^+/\hbar} e^{-ip_0 \sqrt{2m\omega}/4m\hbar} \left| 0 \right> = e^{-p_0^2/2m\hbar} \left| 0 \right> \left| 0 \right> = e^{-p_0^2/2m\hbar}
\]
where we have used
\[
e^{-ip_0 \sqrt{\frac{\hbar}{2m\omega}} a^+/\hbar} \left| 0 \right> = \left| 0 \right>, \quad \left< 0 \right| e^{-ip_0 \sqrt{\frac{\hbar}{2m\omega}} a^+/\hbar} = \left< 0 \right|
\]

### 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 $|z\rangle = e^{z a^+} |0\rangle$.

We have
\[
|z\rangle = e^{z a^+} |0\rangle
\]

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

\[
\hat{a} |z\rangle = \hat{a} e^{z a^+} |0\rangle = \sum_{n=0}^{\infty} \frac{z^n}{n!} \hat{a} (\hat{a}^+)^n |0\rangle = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} (\hat{a}^+)^n |0\rangle
\]

\[
= z \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle = z \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \left( \frac{(\hat{a}^+)^n}{\sqrt{n!}} |0\rangle \right) = z e^{z a^+} |0\rangle = z |z\rangle
\]

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

\[
\langle z_1 | z_2 \rangle = \langle 0 | e^{z_1^* a^+} e^{z_2 a^+} |0\rangle = \left( \sum_{m=0}^{\infty} \frac{z_1^m}{m!} \langle m | \right) \left( \sum_{n=0}^{\infty} \frac{z_2^n}{n!} | n\rangle \right)
\]

\[
= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{z_1^n}{m!} \frac{z_2^m}{n!} \frac{z_1^m}{\sqrt{m!}} \frac{z_2^n}{\sqrt{n!}} \delta_{mn}
\]

\[
= \sum_{n=0}^{\infty} \frac{z_1^n}{\sqrt{n!}} \frac{z_2^n}{n!} = e^{z_1^* z_2};
\]

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(c) Show that the completeness relation takes the form
\[
\int \frac{dx\,dy}{\pi} \langle z | e^{-z^*z} z\rangle = \int \frac{dx\,dy}{\pi} e^{z\hat{a}^+} |0\rangle \langle 0| e^{z^*\hat{a}} e^{-z^*z} \\
= \sum_{m,n} \int \frac{dx\,dy}{\pi} \frac{z^m (\hat{a}^+)^m}{m!} \frac{(z^*)^n (\hat{a})^n}{n!} e^{-z^*z} \\
= \sum_{m,n} \int_0^{2\pi} \frac{d\phi}{\pi} \int_0^\infty rdr \frac{r^m e^{in\varphi} (\hat{a}^+)^m}{m!} |0\rangle \langle 0| \frac{r^n e^{-in\varphi} (\hat{a})^n}{n!} e^{-r^2}
\]
where we have used \( z = re^{i\varphi} \). Now
\[
\int_0^{2\pi} \frac{d\phi}{\pi} e^{i(m-n)\varphi} = 2\delta_{mn}
\]
Therefore, doing the \( m \) sum we have
\[
\int \frac{dx\,dy}{\pi} \langle z | e^{-z^*z} z\rangle = \sum_n \frac{1}{n!} \int_0^\infty rr^{2n} e^{-r^2} dr \left( \frac{(\hat{a}^+)^n}{\sqrt{n!}} \right) \left( \frac{(\hat{a})^n}{\sqrt{n!}} \right) \\
= \sum_n \frac{1}{n!} \int_0^\infty rr^{2n} e^{-r^2} dr \langle |n\rangle \langle n| \rangle = \sum_n |n\rangle \langle n| \frac{1}{n!} \int_0^\infty rr^{2n} e^{-r^2} dr
\]
Now using \( r^2 = x \) we have
\[
\int_0^\infty rr^{2n} e^{-r^2} dr = \int_0^\infty x^n e^{-x} dx = n!
\]
so that
\[
\int \frac{dx\,dy}{\pi} \langle z | e^{-z^*z} z\rangle = \sum_n |n\rangle \langle n| = \hat{I}
\]
This unusual form of the completeness relation reflects the fact that the coherent states form an overcomplete set of states.
\[
\hat{I} = \sum_n |n\rangle \langle n| = \int \frac{dx\,dy}{\pi} \langle z | e^{-z^*z} z\rangle
\]
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.

Since $V(x) = V(-x)$, we have parity conservation and thus only even and odd eigenfunctions. The delta function term in Schrodinger’s equation is proportional to $\psi(0) \delta(x)$, which vanishes for any odd function that satisfies the rest of the equation, such as harmonic oscillator odd eigenfunctions. Thus, the odd eigenfunction of the harmonic oscillator alone are still eigenfunctions of the new Hamiltonian.

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

We have

$$\psi_E(x) = \sum_{\nu=0}^{\infty} C_{2\nu} \psi_{2\nu}(x)$$

where the even eigenfunctions of the harmonic oscillator satisfy

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_{2\nu}(x) + \frac{1}{2} m \omega^2 x^2 \psi_{2\nu}(x) = E_{2\nu} \psi_{2\nu}(x) = \hbar \omega (2\nu + 1/2) \psi_{2\nu}(x)$$

The new Schrodinger equation is then

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_{2\nu}(x) + \frac{1}{2} m \omega^2 x^2 \psi_E(x) - E \psi_E(x) = -\frac{\hbar^2 g}{2m} \psi_E(0) \delta(x)$$

$$\sum_{\nu=0}^{\infty} C_{2\nu} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 - E\right) \psi_{2\nu}(x) = -\frac{\hbar^2 g}{2m} \psi_E(0) \delta(x)$$

$$\sum_{\nu=0}^{\infty} C_{2\nu} \left(\hbar \omega \left(2\nu + \frac{1}{2}\right) - E\right) \psi_{2\nu'}(x) = -\frac{\hbar^2 g}{2m} \psi_E(0) \delta(x)$$

Multiplying by $\psi_{2\nu'}(x)$ and integrating gives, owing to the orthonormality of the harmonic oscillator eigenfunctions (remember they are real)

$$\left(\hbar \omega \left(2\nu' + \frac{1}{2}\right) - E\right) C_{2\nu'} = -\frac{\hbar^2 g}{2m} \psi_E(0) \psi_{2\nu'}(0)$$

or

$$C_{2\nu} = -\frac{\hbar^2 g}{2m} \frac{\psi_E(0) \psi_{2\nu}(0)}{\hbar \omega \left(2\nu + \frac{1}{2}\right) - E}$$
(c) Show that the energy eigenvalues that correspond to even eigenstates are solutions of the equation

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

You might need the fact that

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

Substituting into the expansion of $\psi_E(x)$ we obtain

$$\psi_E(x) = \sum_{\nu=0}^{\infty} C_{2\nu} \psi_{2\nu}(x) = -\frac{\hbar^2 g}{2m} \psi_E(0) \sum_{\nu=0}^{\infty} \frac{\psi_{2\nu}(0)}{\hbar\omega (2\nu + \frac{1}{2}) - E}$$

At the point $x = 0$, this expression is true provided that

$$\frac{1}{g} = -\frac{\hbar^2}{2m} \sum_{\nu=0}^{\infty} \frac{|\psi_{2\nu}(0)|^2}{\hbar\omega (2\nu + \frac{1}{2}) - E}$$

Using the given values of $\psi_{2\nu}(0)$, this is equivalent to

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

(d) Using the given gamma function expression we get 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.

Using the given gamma function expression we get
\[
\frac{4}{g} = -\sqrt{\frac{h}{m\omega}} \frac{\Gamma(1/4 - E/2h\omega)}{\Gamma(3/4 - E/2h\omega)}
\]

The right-hand side has poles at the points
\[
\frac{1}{4} - \frac{E}{2h\omega} = -n , \quad n = 0, 1, 2, ... \Rightarrow E = h\omega \left( \frac{2n}{2} + \frac{1}{2} \right)
\]
and zeroes at the points
\[
\frac{3}{4} - \frac{E}{2h\omega} = -n , \quad n = 0, 1, 2, ... \Rightarrow E = h\omega \left( \frac{2n}{2} + \frac{3}{2} \right)
\]

we have for \( z = -\varepsilon \), with \( \varepsilon > 0 \)
\[
\Gamma(-\varepsilon) = -\frac{\Gamma(1-\varepsilon)}{\varepsilon} = -\frac{\Gamma(1)}{\varepsilon} = -\frac{1}{\varepsilon} < 0
\]

For \( E > 0 \), the right-hand side can be plotted as shown below.

Figure 8.4: Plot of \( \frac{\Gamma(1/4-x)}{\Gamma(3/4-x)} \)
For $g > 0$, the LHS is the horizontal line in the lower half-plane cutting an infinity of points

$$E_\nu < \hbar \omega \left(2\nu + \frac{1}{2}\right)$$

Thus, the positive energy eigenvalues are in one-to-one correspondence with those of the even harmonic oscillator eigenfunctions, lying lower or higher than them in the repulsive or attractive delta function case respectively.

In the attractive case ($g < 0$) there is also a single negative energy eigenstate. For $E = -|E| < 0$, the RHS of

$$-4g \sqrt{\frac{m\omega}{\hbar}} = \frac{\Gamma(1/4 + |E|/2\hbar\omega)}{\Gamma(3/4 + |E|/2\hbar\omega)}$$

is a monotonic function of $|E|$ that starts from the value

$$\frac{\Gamma(1/4)}{\Gamma(3/4)} \approx 2.96$$

at $E = 0$ and decreases to 1 at $|E| \to \infty$. The LHS is a horizontal line. There is a single solution, provided that the coupling is such that

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

### 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)?

For the system initially prepared in the ground-state, we have

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{a}} \cos \left(\frac{\pi x}{a}\right) & |x| \leq a/2 \\ 0 & |x| \geq a/2 \end{cases}$$

The possible values one can measure for any observable are its eigenvalues, say $\alpha$, with probability

$$P_\alpha = |\langle \alpha | \psi \rangle|^2$$

(i) **Energy**: $\psi(x)$ is an energy eigenfunction (ground-state with $n = 1$). This implies that we have only one possible value for the energy, namely, the corresponding eigenvalue

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$$
with probability = 1.

(ii) Position: The possible values are between \(-a/2 \leq x \leq +a/2\) with the probability density

\[
P(x) = \begin{cases} \frac{2}{a} \cos^2 \left( \frac{\pi x}{a} \right) & |x| \leq a/2 \\ 0 & |x| \geq a/2 \end{cases}
\]

(iii) Momentum: The momentum eigenfunctions are plane waves (since the energy is all kinetic energy for a particle in the well)

\[u_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}\]

with eigenvalue \(p = \hbar k\). The probability density for different \(k\) values is given by

\[P(k) = \left| \tilde{\psi}(k) \right|^2\]

where

\[\tilde{\psi}(k) = \langle u_k | \psi \rangle = \int_{-\infty}^{\infty} dx \frac{dx}{\sqrt{2\pi}} e^{-ikx} \psi(x)\]

which is the Fourier transform of the position space wave function. The momentum space wave function is defined by

\[\tilde{\varphi}(p) = \frac{1}{\sqrt{\hbar}} \tilde{\psi}(k = p/\hbar)\]

Note that an alternative form for the position space wave function is

\[
\psi(x) = \sqrt{\frac{2}{a}} \cos \left( \frac{\pi x}{a} \right) \theta(x) \quad \text{all } x \quad \text{where} \quad \theta(x) = \begin{cases} 1 & |x| \leq a/2 \\ 0 & |x| \geq a/2 \end{cases}
\]

Method #1: Fourier Transform
Using the first form of the wave function we get

\[ \tilde{\psi}(k) = \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx = \sqrt{\frac{a}{2}} \int_{-a/2}^{a/2} \cos \left( \frac{\pi x}{a} \right) e^{-ikx} dx = \frac{1}{2} \sqrt{\frac{a}{2}} \int_{-a/2}^{a/2} \left( e^{i\pi x/a} + e^{-i\pi x/a} \right) e^{-ikx} dx \]

\[ = \frac{1}{2} \sqrt{\frac{a}{2}} \int_{-a/2}^{a/2} \left( e^{i(\pi/a-k)x} + e^{-i(\pi/a+k)x} \right) dx \]

\[ = \frac{1}{2} \sqrt{\frac{a}{2}} \int_{-a/2}^{a/2} e^{y} dy + \frac{1}{2} \sqrt{\frac{a}{2}} \int_{-a/2}^{a/2} e^{-y} dy \]

\[ = \frac{1}{2} \sqrt{\frac{a}{2}} \left( -2i \sin(\pi/a-k)a/2 \right) + \frac{1}{2} \sqrt{\frac{a}{2}} \left( -2i \sin(\pi/a+k)a/2 \right) \]

\[ = \sqrt{\frac{a}{2}} \left[ \text{Sinc} \left( \frac{ka}{2} - \frac{\pi}{2} \right) + \text{Sinc} \left( \frac{ka}{2} - \frac{\pi}{2} \right) \right] \]

**Method #2: Fourier Transform**

Using the second form of the wave function and the convolution rule below.

For

\[ A(x) = B(x)C(x) \]

with

\[ \tilde{A}(k) = \int_{-\infty}^{\infty} A(x) e^{-ikx} dx \]
\[ \tilde{B}(k) = \int_{-\infty}^{\infty} B(x) e^{-ikx} dx \]

and

\[ \tilde{C}(k) = \int_{-\infty}^{\infty} C(x) e^{-ikx} dx \]

we have

\[ \tilde{A}(k) = \tilde{B}(k) \ast \tilde{C}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq \tilde{B}(q) \tilde{C}(k-q) \]

We have to find

\[ \tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx \]

where

\[ \psi(x) = \sqrt{\frac{a}{2}} \cos \left( \frac{\pi x}{a} \right) \theta(x) \]
Defining

\[ B(x) = \sqrt{\frac{2}{a}} \cos \left( \frac{\pi x}{a} \right) \]

we have

\[ \tilde{B}(k) = \int_{-\infty}^{\infty} \sqrt{\frac{2}{a}} \cos \left( \frac{\pi x}{a} \right) e^{-ikx} dx = \frac{1}{2} \sqrt{\frac{2}{a}} \int_{-\infty}^{\infty} (e^{i\pi x/a} + e^{-i\pi x/a}) e^{-ikx} dx \]

\[ = \frac{1}{2} \sqrt{\frac{2}{\pi}} \sqrt{2\pi} [\delta(k - \pi/a) + \delta(k + \pi/a)] \]

These two delta functions correspond to a standing wave which is the superposition of \( e^{ip_1x/\hbar} \) and \( e^{-ip_1x/\hbar} \) where \( p_1 = \pi/a \).

Now defining

\[ C(x) = \theta(x) \]

we have

\[ \tilde{C}(k) = \int_{-\infty}^{\infty} \theta(x)e^{-ikx} dx = \int_{-a/2}^{a/2} e^{-ikx} dx = \frac{2}{k} \sin \frac{ka}{2} = aSinc \left( \frac{ka}{2} \right) \]

and then we have

\[ \tilde{A}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq \tilde{B}(q)\tilde{C}(k-q) \]

\[ = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a}} \sqrt{2\pi} \int_{-\infty}^{\infty} dq [\delta(q - \pi/a) + \delta(q + \pi/a)]Sinc \left( \frac{(k-q)a}{2} \right) \]

\[ = \sqrt{\frac{a}{2}} \left[ Sinc \left( \frac{ka}{2} - \frac{\pi}{2} \right) + Sinc \left( \frac{ka}{2} - \frac{\pi}{2} \right) \right] = \tilde{\psi}(k) \]

which is the same as the first result. This looks like
The dotted curves are the two \( \text{Sinc} \) functions. The huge spread is due to strong localization in \( x \), that is, because the particle is localized, we get uncertainty in momentum beyond the two delta function spikes.

With
\[
\tilde{\phi}(p) = \frac{1}{\sqrt{\hbar}} \tilde{\psi}(k = p/\hbar)
\]

we have any value \(-\infty < p < +\infty\) where the probability density is
\[
P(p) = |\tilde{\phi}(p)|^2
\]

(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?

Now the particle is measured to be near \( x = 0 \), but we are completely uncertain within the range \(-a/4 \leq x \leq +a/4\). A reasonable post-measurement state assignment is then
\[
\psi_+(x) = \begin{cases} \sqrt{\frac{2}{a}} & -a/4 < x < a/4 \\ 0 & \text{otherwise} \end{cases}
\]

as shown below.
Note that we have completely thrown away our prior information. This might not always be the best strategy to get good predictions.

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

To find the possibilities for measurement outcomes, we must expand $\psi_+(x)$ in the eigenfunctions of that observable.

**Energy Eigenfunctions:**

$$\psi_+(x) = \sum_n c_n u_n(x)$$

where

$$u_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \cos \frac{n\pi x}{a} & n = 1, 3, 5, \ldots, \\ \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} & n = 2, 4, 6, \ldots. \end{cases}$$

and so

$$c_n = \int_{-a/4}^{a/4} dx \, u_n^* (x) \psi_+ (x) = \langle u_n | \psi_+ \rangle$$

Since $\psi_+(x)$ is an even function, only the cosine terms survive. Thus, for $n = 1, 3, 5, \ldots$

$$c_n = \sqrt{\frac{2}{a}} \sqrt{\frac{2}{a}} \int_{-a/4}^{a/4} \cos \frac{n\pi x}{a} dx = \frac{2}{n\pi} \left( \sin \frac{n\pi}{4} - \sin \frac{-n\pi}{4} \right) = \frac{4}{n\pi} \sin \frac{n\pi}{4} \quad n = 1, 3, 5, 7, \ldots$$

and therefore, the possible energies are

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad n = 1, 3, 5, \ldots$$
with probability

$$|c_n|^2 = \frac{16}{n^2\pi^2} \sin^2 \frac{n\pi}{4} = \frac{8}{n^2\pi^2} \quad n = 1, 3, 5, 7, \ldots.$$ 

**Possible Positions**: Any value in the range $$-a/4 \leq x \leq +a/4$$ with a uniform probability density

$$P(x) = \frac{2}{a}$$

**Momentum**: We have the momentum wave function

$$\hat{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi_+(x)e^{-ipx/\hbar}dx$$

This implies that

$$\hat{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{2}{a}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}dx = \frac{1}{\sqrt{\pi\hbar a}} \left( e^{-ipa/4\hbar} - e^{ipa/4\hbar} - i p/\hbar \right)$$

Thus, we have a continuum of momentum values from $$-\infty < p < +\infty$$ with the probability density

$$|\hat{\phi}(p)|^2 = \frac{a}{4\pi\hbar} \text{sinc}^2 \left( \frac{pa}{4\hbar} \right)$$

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

I do not think anything changes!

### 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 Figure 8.5 below).
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 $I \neq 0$.

In the presence of a vector potential $\vec{A}$, minimal coupling says that

$$\vec{p} \rightarrow \vec{p} - \frac{e}{c}\vec{A}$$

Now, in the absence of an EM-field, the Schrodinger equation is

$$i\hbar \frac{\partial \psi_0(\vec{r}, t)}{\partial t} = \left[ \frac{1}{2m}\vec{p}^2 + V(\vec{r}) \right] \psi_0(\vec{r}, t)$$

Adding an EM-field implies that

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = \left[ \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - +V(\vec{r}) \right] \psi(\vec{r}, t)$$

where $\nabla \times \vec{A} = \vec{B}$.

If we let

$$\psi(\vec{r}, t) = \psi_1(\vec{r}, t)e^{\frac{i}{\hbar} \int_{\vec{r}}^{\vec{r}'} \vec{A} \cdot d\vec{r}}$$

where the integral signifies any path ending at $\vec{r}'$, then $\psi_1(\vec{r}, t)$ satisfies the Schrodinger equation with no EM-field ($I = 0$). Therefore,

$$\psi_1(\vec{r}, t) = \psi_0(\vec{r}, t) = \psi_0(\vec{r})e^{-iEt/\hbar}$$

so that

$$\psi(\vec{r}, t) = \psi_0(\vec{r})e^{-iEt/\hbar}e^{\frac{i}{\hbar} \int_{\vec{r}}^{\vec{r}'} \vec{A} \cdot d\vec{r}}$$
(b) Consider the two-slit diffraction experiment for the particles described above shown in Figure 8.5 above. Assume that the distance $d$ between the two slits is large compared to the diameter of the solenoid.

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

When $I = 0$, for any point on the screen, the probability amplitude is

$$f = f_+ + f_-$$

where

$$f_+ = \text{amplitude from upper slit path}$$
$$f_- = \text{amplitude from lower slit path}$$

When $I \neq 0$, we then have

$$f' = f'_+ + f'_-$$

where

$$f'_+ = f_+ e^{i \oint_{C_+} \frac{\varepsilon}{c} \vec{A} \cdot d\vec{r}}$$
$$f'_- = f_- e^{i \oint_{C_-} \frac{\varepsilon}{c} \vec{A} \cdot d\vec{r}}$$

$C_+$ corresponds to the upper path and $C_-$ corresponds to the lower path.

Therefore,

$$f' = f'_+ + f'_- = f_+ e^{i \oint_{C_+} \frac{\varepsilon}{c} \vec{A} \cdot d\vec{r}} + f_- e^{i \oint_{C_-} \frac{\varepsilon}{c} \vec{A} \cdot d\vec{r}} \propto f_+ + f_- e^{i \oint_{C_-} \frac{\varepsilon}{c} \vec{A} \cdot d\vec{r} - \oint_{C_+} \frac{\varepsilon}{c} \vec{A} \cdot d\vec{r}}$$

or

$$f' \propto f_+ + f_- e^{i \oint \frac{\varepsilon}{c} \vec{A} \cdot d\vec{r}}$$

where the closed path integral is CCW along an arbitrary path surrounding the solenoid.

This says that the solenoid adds a phase factor

$$\frac{e\varphi}{\hbar c} = \frac{e}{\hbar c} \oint \vec{A} \cdot d\vec{r}$$

to the probability amplitudes at points on the screen (due to lower slit).

Remembering approximations in Young’s interference (in optics) we get that the interference pattern is shifted by $\Delta s$, where assuming that $L \gg d$ and $L \gg \Delta s$, we find

$$\frac{\Delta s}{d} \propto \frac{e\varphi L}{\hbar c dk} = \text{phase shift}$$

$$\Delta s = \frac{e\varphi L}{\hbar c dk} \gg \frac{e\varphi L}{\hbar c d \sqrt{2mE_0}}$$
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 $\psi_i$, $i = 1, 2$ of the two wires can be characterized by the numbers $n_i$ of Cooper pairs (charge $= -2e$) and phases $\theta_i$, 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 so-called Josephson energy. The interesting physics is expressed in terms of the differences

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

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

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

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

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

The terms in these equations represent the following processes. First consider the first term on the RHS or the direct term:

$$U_1 \psi_1$$

which just gives a solution of the form $e^{i\omega t}$ representing steady-state behavior of the probability amplitude on side #1 and similarly for side #2. The second term on the RHS or the tunneling term

$$\frac{E_J}{n_0} \psi_2$$

represents a probability current flow across the boundary between regions, i.e., change in region one due to current proportional to amplitude on side #2 and similar for the other side.
(b) Using \( \psi_i = \sqrt{n_i}e^{i\theta_i} \), show that the equations of motion for \( n \) and \( \varphi \) are given by

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

Using \( \psi_i = \sqrt{n_i}e^{i\theta_i} \), we find

\[
\begin{align*}
\text{i} \hbar \left( \frac{\dot{n}_1}{\sqrt{n_1}} e^{i\theta_1} + \text{i} \dot{\theta}_1 \sqrt{n_1} e^{i\theta_1} \right) &= -\frac{ne^2}{C} \sqrt{n_1} e^{i\theta_1} - \frac{E_J}{n_0} \sqrt{n_2} e^{i\theta_2} \\
\text{i} \hbar \left( \frac{\dot{n}_2}{\sqrt{n_2}} e^{i\theta_2} + \text{i} \dot{\theta}_2 \sqrt{n_2} e^{i\theta_2} \right) &= \frac{ne^2}{C} \sqrt{n_2} e^{i\theta_2} - \frac{E_J}{n_0} \sqrt{n_1} e^{i\theta_1}
\end{align*}
\]

or

\[
\begin{align*}
\text{i} \hbar \frac{\dot{n}_1}{n_1} - \hbar \dot{\theta}_1 &= -\frac{ne^2}{C} n_1 - \frac{E_J}{n_0} \sqrt{n_1 n_2} e^{i\varphi} \\
\text{i} \hbar \frac{\dot{n}_2}{n_2} - \hbar \dot{\theta}_2 &= \frac{ne^2}{C} n_2 - \frac{E_J}{n_0} \sqrt{n_1 n_2} e^{-i\varphi}
\end{align*}
\]

Taking real and imaginary parts,

\[
\begin{align*}
\dot{\theta}_1 &= \frac{ne^2}{C} + \frac{E_J}{n_0} \sqrt{n_2} \cos \varphi \\
\dot{n}_1 &= -\frac{E_J}{n_0} \sqrt{n_1 n_2} \sin \varphi \\
\dot{\theta}_2 &= \frac{ne^2}{C} + \frac{E_J}{n_0} \sqrt{n_1} \cos \varphi \\
\dot{n}_2 &= \frac{E_J}{n_0} \sqrt{n_1 n_2} \sin \varphi
\end{align*}
\]

Taking differences, we find the equations for \( n \) and \( \varphi \),

\[
\begin{align*}
\dot{\varphi} &= \dot{\theta}_2 - \dot{\theta}_1 \approx -\frac{2ne^2}{\hbar C} - \frac{E_J}{n_0} \left( \sqrt{n_2} - \sqrt{n_1} \right) \cos \varphi \approx -\frac{2ne^2}{\hbar C} \\
\dot{n} &= \dot{n}_2 - \dot{n}_1 \approx \frac{2E_J}{n_0} \sqrt{n_1 n_2} \sin \varphi \approx \frac{E_J}{\hbar} \sin \varphi
\end{align*}
\]

noting that \( n_1 \approx n_2 \approx n_0/2 \). Taking the sums, we find that \( n = \text{constant} \).

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

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

We identify a pair(electrical) current from side 1 to side 2

\[
J_S = (-2e) \frac{\dot{n}}{2} = -\frac{eE_J}{\hbar} \sin \varphi \equiv J_0 \sin \varphi
\]

where the maximum current is

\[
J_0 = \frac{eE_J}{\hbar} = \frac{2\pi e E_J}{\hbar} = \frac{\pi E_J}{\phi_0}
\]

(d) Show that

\[
\dot{\varphi} \approx -\frac{2e^2 E_J}{\hbar^2 C} \sin \varphi
\]

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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 $\varphi = \pi$.

We can exhibit oscillatory behavior as follows. We have

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

If $E_J$ is positive, then 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 $\varphi = \pi$, since $\sin(\pi - \varphi) = \sin \varphi$ while $d^2(\pi - \varphi)/dt^2 = -\ddot{\varphi}$. The frequency of oscillation is the same as above now using $|E_J|$.

(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

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

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

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

We have

$$\dot{\varphi} = -\frac{2ne^2}{\hbar C} = -\frac{2VCe}{\hbar C} = -\frac{2eV}{\hbar} = -\omega$$
which implies that $\varphi = -\omega t$

$$
J_S = \epsilon \hbar = C\dot{V} = -C\frac{\hbar}{2e} \dot{\varphi} = -C\frac{\hbar}{2e} \left( -\frac{2e^2E_j}{\hbar^2C} \sin \omega t \right) = J_0 \sin \omega t
$$

where

$$
J_0 = \frac{C\hbar 2e^2E_j}{2e \hbar^2C} = \frac{eE_j}{\hbar}
$$

### 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.

Let us transform to a new set of operators

$$
\hat{a} = \hat{b} + \alpha , \quad \hat{a}^+ = \hat{b}^+ + \alpha^*
$$

Simple algebra show they have the same commutation relations, i.e.,

$$
[\hat{a}, \hat{a}^+] = 1 = [\hat{b}, \hat{b}^+]
$$

Therefore they both have the same eigenvector/eigenvalue structure, i.e.,

$$
\hat{a}^+ \hat{a} |n\rangle_a = n |n\rangle_a \quad n = 0, 1, 2, 3, 4,.....
$$

$$
\hat{b}^+ \hat{b} |n\rangle_b = n |n\rangle_b \quad n = 0, 1, 2, 3, 4,.....
$$

Substituting into the Hamiltonian we have

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

If we choose $\alpha = -V^*$, we get

$$
\hat{H} = \hbar \omega \hat{b}^+ \hat{b} - |V|^2
$$

Therefore,

$$
\hat{H} |n\rangle_b = (\hbar \omega n - |V|^2) |n\rangle_b
$$

Thus, the energy eigenvalues are

$$
E_n = \hbar \omega n - |V|^2 \quad n = 0, 1, 2,.....
$$

The ground state of the system corresponds to $\hat{b} |0\rangle_b$ with ground state energy $E_0 = -|V|^2$. We also have

$$
\hat{b} |0\rangle_b = 0 = (\hat{a} + \alpha) |0\rangle_b = 0 \rightarrow \hat{a} |0\rangle_b = \alpha |0\rangle_b = -V^* |0\rangle_b
$$

The ground state is a coherent state.
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
\[
\hat{H} = \hbar \omega \hat{a}^+ \hat{a} + \frac{1}{2} V (\hat{a} \hat{a}^+ + \hat{a}^+ \hat{a})
\]
(There is an upper limit on \(V\) for which this can be done). Also show that the unitary operator
\[
\hat{U} = e^{(\hat{a} \hat{a} + \hat{a}^+ \hat{a}^+)} \eta / 2
\]
can relate the two sets of operators as \(\hat{b} = \hat{U} \hat{a} \hat{U}^{-1}\).

We have
\[
\hat{b} = \hat{a} \cosh \eta + \hat{a}^+ \sinh \eta \\
\hat{b}^+ = \hat{a}^+ \cosh \eta + \hat{a} \sinh \eta
\]
Now using \([\hat{a}, \hat{a}^+] = 1\) we get
\[
[\hat{b}, \hat{b}^+] = \left[ \hat{a} \cosh \eta + \hat{a}^+ \sinh \eta, \hat{a}^+ \cosh \eta + \hat{a} \sinh \eta \right]
= \cosh^2 \eta [\hat{a}, \hat{a}^+] - \sinh^2 \eta [\hat{a}, \hat{a}^+]
= \cosh^2 \eta - \sinh^2 \eta = 1
\]
so that the commutation relations are preserved.

We also have
\[
\hat{a} = \hat{b} \cosh \eta - \hat{b}^+ \sinh \eta \\
\hat{a}^+ = \hat{b}^+ \cosh \eta - \hat{b} \sinh \eta
\]
Therefore,
\[
\hat{H} = \hbar \omega (\hat{b}^+ \cosh \eta - \hat{b} \sinh \eta) (\hat{b} \cosh \eta - \hat{b}^+ \sinh \eta)
+ \frac{V}{2} ((\hat{b} \cosh \eta - \hat{b}^+ \sinh \eta)^2 + (\hat{b}^+ \cosh \eta - \hat{b} \sinh \eta)^2)
= \hbar \omega (\hat{b}^+ \hat{b} \cosh^2 \eta - (\hat{b}^+)^2 \cosh \eta \sinh \eta - \hat{b} \hat{b}^+ \cosh \eta \sinh \eta + \hat{b} \hat{b}^+ \sinh^2 \eta)
+ \frac{V}{2} ((\hat{b}^+)^2 (\cosh^2 \eta + \sinh^2 \eta) + (\hat{b}^+)^2 (\cosh^2 \eta + \sinh^2 \eta)
- \hat{b} \hat{b}^+ \cosh \eta \sinh \eta - \hat{b}^+ \hat{b} \cosh \eta \sinh \eta)
\]
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Rearranging and using $[\hat{b}, \hat{b}^+] = 1$ we get

\[
\hat{H} = (\hbar \omega (\cosh^2 \eta + \sinh^2 \eta) - 2V \cosh \eta \sinh \eta) \hat{b}^+ \hat{b} \\
+ (-\hbar \omega \cosh \eta \sinh \eta + V (\cosh^2 \eta + \sinh^2 \eta)/2)((\hat{b}^+)^2 + (\hat{b})^2) \\
+ \hbar \omega \sinh^2 \eta - V \cosh \eta \sinh \eta
\]

Now using

\[
\sinh 2\eta = 2 \cosh \eta \sinh \eta , \quad \cosh^2 \eta + \sinh^2 \eta = 1
\]

we can eliminate the squared operator terms by the choice

\[ V = \hbar \omega \tanh 2\eta \]

We then have

\[
\hat{H} = \Omega \hat{b}^+ \hat{b} + F
\]

where

\[
\Omega = \hbar \omega \cosh 2\eta - V \sinh 2\eta \\
F = \hbar \omega \sinh^2 \eta - V \cosh \eta \sinh \eta
\]

Thus the energy eigenvalues are

\[ E_n = \Omega n + F \quad n = 0, 1, 2, \ldots \]

Now the coefficient of $n$ must be $> 0$ to make physical sense (energy would go to $-\infty$). This says that

\[ \Omega > 0 \rightarrow V < \frac{\hbar \omega}{\tanh 2\eta} = \frac{(\hbar \omega)^2}{V} \]

which says that we must have

\[ V < \hbar \omega \]

Finally, for $\hat{U} = e^{(\hat{a} \hat{a} + \hat{a}^+ \hat{a}^+)/2}$ and using

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

with $A = (\hat{a} \hat{a} + \hat{a}^+ \hat{a}^+)/2$ and using

\[ [\hat{a}^+ \hat{a}^+, \hat{a}] = -2\hat{a}^+ , \quad [\hat{a} \hat{a}, \hat{a}^+] = 2\hat{a} \]

we have

\[ \hat{U} \hat{a} \hat{U}^{-1} = \hat{a} \left( 1 + \frac{\eta^2}{2!} + \ldots \right) - \hat{a}^+ \hat{a} \left( \eta + \frac{\eta^3}{3!} + \ldots \right) \]

or

\[ \hat{a} = \hat{b} \cosh \eta - \hat{b}^+ \sinh \eta \]

as before.
8.15.20 Harmonic oscillator

Consider a particle in a 1-dimensional harmonic oscillator potential. Suppose at time \( t = 0 \), the state vector is

\[ |\psi(0)\rangle = e^{-\frac{ia}{\hbar}} |0\rangle \]

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 \( \hat{x}(t) \).

We first determine the position operator \( x(t) \) in the Heisenberg representation. Using \( [x, \hat{p}] = i\hbar \) gives the operator equations of motion

\[
\dot{x}(t) = \frac{i}{\hbar} [H, x] = \frac{i}{\hbar} \frac{1}{2m} (\hat{p}\hat{x} - \hat{x}\hat{p}) = \frac{i}{\hbar} \frac{1}{2m} (-2i\hbar \hat{p}) = \frac{p(t)}{m} \\
\dot{p}(t) = \frac{i}{\hbar} [H, \hat{p}] = \frac{i}{\hbar} m\omega^2 (\hat{x}\hat{p} - \hat{p}\hat{x}) = \frac{i}{\hbar} m\omega^2 (2i\hbar x) = -m\omega^2 x(t)
\]

The solution of these equations is

\[ x(t) = x \cos \omega t + \frac{p}{m\omega} \sin \omega t \]

(same as classical problem!) where \( x = x(0), p = p(0) \) are Schrödinger operators.

(b) Show that \( e^{-\frac{ia}{\hbar}} \) is the translation operator.

See Problem 6.19.2. We then have

\[ T(a) |a\rangle = e^{-ipa/\hbar} |x\rangle = |x + a\rangle \]

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

We have

\[
\langle x \rangle = \langle 0 | e^{ipa/\hbar} x(t) e^{-ipa/\hbar} |0 \rangle = \langle 0 | \hat{I} e^{ipa/\hbar} x(t) e^{-ipa/\hbar} \hat{I} |0 \rangle \\
= \int dx' \int dx'' \langle 0 | x' \rangle \langle x' | e^{ipa/\hbar} x(t) | x'' \rangle \langle x'' | 0 \rangle \\
= \int dx' \int dx'' \langle 0 | x' \rangle \langle x' + a | x'' + a \rangle (x \cos \omega t + \frac{p}{m\omega} \sin \omega t) | x'' + a \rangle \langle x'' | 0 \rangle \\
= \int dx' \int dx'' \langle 0 | x' \rangle \langle x' + a | ((x'' + a) \cos \omega t) | x'' + a \rangle \langle x'' | 0 \rangle
\]

where the \( p \)-term vanishes since

\[ \langle 0 | e^{ipa/\hbar} p e^{-ipa/\hbar} |0 \rangle = \langle 0 | p |0 \rangle = 0 \]

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Now use
\[ \int dx' \langle x'' + a | x'' + a \rangle = 1 \]
to get
\[ \langle x \rangle = \int dx \langle 0 | x + a \rangle \cos \omega t \langle x | 0 \rangle = a \cos \omega t \]
since \( \langle 0 | 0 \rangle = 1, \langle 0 | x | 0 \rangle = 0. \) This answer is natural since it corresponds to the position of an initially displaced particle in a harmonic potential.

8.15.21 Another oscillator

A 1-dimensional harmonic oscillator is, at time \( t = 0, \) in the state
\[ |\psi(t = 0)\rangle = \frac{1}{\sqrt{3}} (|0\rangle + |1\rangle + |2\rangle) \]
where \( |n\rangle \) is the \( n^{th} \) energy eigenstate. Find the expectation value of position and energy at time \( t. \)

We have the state vector at time \( t: \)
\[ |\psi(t)\rangle = \frac{1}{\sqrt{3}} \left( e^{-iE_0 t/\hbar} |0\rangle + e^{-iE_1 t/\hbar} |1\rangle + e^{-iE_2 t/\hbar} |2\rangle \right) \]
where \( E_n = \hbar \omega (n + 1/2). \) Using \( \langle i | j \rangle = \delta_{ij} \) the expectation value of the energy becomes
\[ \langle E(t) \rangle = \frac{1}{3} (E_0 + E_1 + E_2) = \frac{3}{2} \hbar \omega \]
which is independent of \( t. \)

For position we have
\[ \langle x(t) \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle \psi | (a + a^+) | \psi \rangle \]
\[ = \frac{1}{3} \sqrt{\frac{\hbar}{2m\omega}} \left( e^{iE_0 t/\hbar} \langle 0 | 0 \rangle + e^{iE_1 t/\hbar} \langle 1 | 1 \rangle + e^{iE_2 t/\hbar} \langle 2 | 2 \rangle \right) (a + a^+) \left( e^{-iE_0 t/\hbar} |0\rangle + e^{-iE_1 t/\hbar} |1\rangle + e^{-iE_2 t/\hbar} |2\rangle \right) \]
\[ = \frac{1}{3} \sqrt{\frac{\hbar}{2m\omega}} \left( e^{i(E_0-E_1) t/\hbar} \langle 0 | a | 1 \rangle + e^{i(E_1-E_2) t/\hbar} \langle 1 | a | 2 \rangle + e^{i(E_1-E_0) t/\hbar} \langle 1 | a | 0 \rangle + e^{i(E_2-E_1) t/\hbar} \langle 2 | a | 1 \rangle \right) \]
\[ = \frac{1}{3} \sqrt{\frac{\hbar}{2m\omega}} \left( e^{-i\omega t} + e^{-i\omega t} \sqrt{2} + e^{i\omega t} + e^{i\omega t} \sqrt{2} \right) = \frac{1}{3} \sqrt{\frac{\hbar}{2m\omega}} (1 + \sqrt{2}) \cos \omega t \]
which oscillates with \( t. \)
8.15.22 The coherent state

Consider a particle of mass \( m \) in a harmonic oscillator potential of frequency \( \omega \). 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 \( \alpha \) 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., \( \hat{a} |\alpha\rangle = \alpha |\alpha\rangle \).

\[
\hat{a} |\alpha\rangle = \sum_{n=0}^{\infty} c_n \hat{a} |n\rangle = \sum_{n=0}^{\infty} c_n \sqrt{n} |n-1\rangle = \sum_{n=0}^{\infty} c_{n+1} \sqrt{n+1} |n\rangle
\]

We also have

\[
c_{n+1} \sqrt{n+1} = e^{-|\alpha|^2/2} \frac{\alpha^{n+1} \sqrt{n+1}}{\sqrt{(n+1)!}} = e^{-|\alpha|^2/2} \frac{\alpha^{n+1}}{\sqrt{n!}} = \alpha c_n
\]

This implies that

\[
\hat{a} |\alpha\rangle = \alpha \sum_{n=0}^{\infty} c_n |n\rangle = \alpha |\alpha\rangle
\]

Thus, the coherent state is an eigenstate of the annihilation operator \( (\alpha \) is a complex number).

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

We have

\[
\hat{x} = x_c \left( \hat{a} + \hat{a}^+ \right) \quad x_c = \sqrt{\frac{2\hbar}{m\omega}}
\]

\[
\hat{p} = p_c \left( \hat{a} - \hat{a}^+ \right) \quad p_c = \sqrt{2m\hbar\omega}
\]

Also

\[
\hat{a} |\alpha\rangle = \alpha |\alpha\rangle \rightarrow \langle \alpha | \hat{a}^+ = \alpha^* \langle \alpha |
\]

which implies that

\[
\langle \alpha | \hat{a} |\alpha\rangle = \alpha \langle \alpha | \alpha \rangle = \alpha
\]

\[
\langle \alpha | \hat{a}^+ |\alpha\rangle = \alpha^* \langle \alpha | \alpha \rangle = \alpha^*
\]

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and then
\[
\langle \alpha | \hat{x} | \alpha \rangle = x_c \frac{\alpha + \alpha^*}{2} = x_c \text{Re}(\alpha)
\]
\[
\langle \alpha | \hat{p} | \alpha \rangle = p_c \frac{\alpha - \alpha^*}{2i} = p_c \text{Im}(\alpha)
\]

(c) Show that, in position space, the wave function for this state is
\[
\psi_\alpha(x) = e^{ip_0 x / \hbar} u_0(x - x_0)
\]
where \( u_0(x) \) is the ground state gaussian function and \( (\hat{x}) = x_0 \) and \( (\hat{p}) = p_0 \).

We have
\[
\alpha \langle x | \alpha \rangle = \langle x | \hat{a} | \alpha \rangle = \langle x | \left( \frac{\hat{x}}{x_c} + \frac{i \hat{p}}{p_c} \right) | \alpha \rangle = \left( \frac{x}{x_c} + \frac{\hbar}{p_c} \frac{d}{dx} \right) \langle x | \alpha \rangle
\]
where \( \langle x | \alpha \rangle = \psi_\alpha(x) \). Therefore the ODE we need to solve is
\[
\frac{\hbar}{p_c} \frac{d \psi}{dx} + \frac{x}{x_c} \psi = \alpha \psi
\]
or
\[
\frac{d \psi}{\psi} = \frac{p_c}{\hbar} \left( \alpha - \frac{x^2}{2x_c} \right) dx
\]
which has the solution
\[
\ln \frac{\psi}{\psi_0} = \frac{p_c}{\hbar} \left( \alpha x - \frac{x^2}{2x_c} \right)
\]
or
\[
\psi = \psi_0 e^{\frac{p_c}{\hbar} \left( \alpha x - \frac{x^2}{2x_c} \right)} = \psi_0 e^{ip_0 \text{Im}(\alpha) x / \hbar} e^{\frac{p_c}{\hbar} \left( \text{Re}(\alpha) x - \frac{x^2}{2x_c} \right)}
\]
if we let
\[
\text{Re}(\alpha) = \frac{x_0}{x_c}, \quad \text{Im}(\alpha) = \frac{p_0}{p_c}
\]
we then have
\[
\psi = \psi_0 e^{ip_0 x / \hbar} e^{\frac{p_c}{\hbar} \left( \frac{\text{Re}(\alpha) x}{x_c} - \frac{x^2}{2x_c} \right)}
\]
\[
= \psi_0 e^{ip_0 x / \hbar} e^{-\frac{p_c}{2x_c} x^2 + \frac{\text{Im}(\alpha) x}{x_c}}
\]
\[
= \psi_0 e^{ip_0 x / \hbar} e^{-\frac{\text{Im}(\alpha) x}{x_c}} e^{-\frac{p_c x^2}{2x_c}}
\]
\[
= \psi_0 e^{ip_0 x / \hbar} u(x - x_0)
\]
where \( \langle x \rangle = x_0 \) and \( (\hat{p}) = p_0 \).

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

We have
\[
(\hat{x}) = x_0 = x_c \text{Re}(\alpha) \to \text{Re}(\alpha) = \frac{x_0}{x_c}
\]
and

\[ \langle \hat{p} \rangle = p_0 = p_c \text{Im}(\alpha) \rightarrow \text{Im}(\alpha) = \frac{p_0}{p_c} \]

so that

\[ \alpha = \frac{x_0}{x_c} + \frac{i p_0}{p_c} \]

and \( x_0 \) and \( p_0 \) are the mean position and momentum.

\( \psi_\alpha(x) \) is the wave packet, Gaussian, centered at \( x = x_0 \) with carrier wave momentum \( p_0 \).

The momentum space wave function is the Fourier transform of \( \psi_\alpha(x) \)

\[ \mathcal{F}(\psi_\alpha(x)) = \tilde{\psi}_\alpha(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx \psi_\alpha(x) e^{-ipx/\hbar} \]

We can use the convolution theorem

\[ \tilde{\psi}_\alpha(p) = \mathcal{F}(e^{ip_0x/\hbar}) \otimes \mathcal{F}(u_0(x - x_0)) \]

We have

\[ \mathcal{F}(e^{ip_0x/\hbar}) = \delta(p - p_0) \]

and by the shift property

\[ \mathcal{F}(u_0(x - x_0))e^{-ix_0p/\hbar} \tilde{u}_0(p) \]

Therefore,

\[ \tilde{\psi}_\alpha(p) = e^{-ix_0p_0/\hbar}(e^{-ix_0p/\hbar} \tilde{u}_0(p - p_0)) \]

where the first exponential factor is just an overall phase factor.

In momentum space, \( \tilde{u}_0 \) is centered at \( p_0 \). The mean position appears as a phase in momentum space.

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

This was explicitly done as part of the solution of part(c).
(f) Show that the coherent state is a minimum uncertainty state (with equal uncertainties in \(x\) and \(p\), in characteristic dimensionless units.

The uncertainties are \(\Delta x = \sqrt{\Delta x^2}, \Delta p = \sqrt{\Delta p^2}\), where

\[
\Delta x^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2, \quad \Delta p^2 = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2
\]

We already have \(\langle \hat{x} \rangle = x_c \Re(\alpha)\) and \(\langle \hat{p} \rangle = p_c \Im(\alpha)\). Now

\[
\langle \hat{x}^2 \rangle = \frac{x_c^2}{4} \langle \alpha | (\hat{a}^2 + \hat{a}^+ \hat{a} + \hat{a}^+ \hat{a}^+ - 1) | \alpha \rangle
\]

Using \(\hat{a} | \alpha \rangle = \alpha | \alpha \rangle \rightarrow \langle \alpha | \hat{a}^+ = \alpha^* \langle \alpha |\)

we get

\[
\langle \hat{x}^2 \rangle = \frac{x_c^2}{4} \langle \alpha | (\alpha^2 + \alpha^* \alpha + \hat{a}^+ \hat{a}^+ - 1) | \alpha \rangle
\]

\[
= \frac{x_c^2}{4} (\alpha + \alpha^*)^2 + \frac{x_c^2}{4} = (x_c \Re(\alpha))^2 + \frac{x_c^2}{4}
\]

or

\[
(\Delta x)^2 = \frac{x_c^2}{4} \rightarrow \Delta x = \frac{x_c}{2} = \sqrt{\frac{\hbar}{2mc\omega}}
\]

and similarly

\[
(\Delta p)^2 = \frac{p_c^2}{4} \rightarrow \Delta p = \frac{p_c}{2} = \sqrt{\frac{\hbar m\omega}{2}}
\]

and hence

\[
\Delta x \Delta p = \frac{\hbar}{2}
\]

so that we have a minimum uncertainty wave packet.

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

\[
|\psi(t)\rangle = e^{-i\omega t/2} | \alpha e^{-i\omega t} \rangle
\]

Interpret this result.

At \(t = 0\) we have \(|\psi(0)\rangle = |\alpha\rangle\). Then

\[
|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = \sum_{n=0}^{\infty} c_n \hat{U}(t) |n\rangle
\]

\[
= \sum_{n=0}^{\infty} c_n e^{-iE_n t/\hbar} |n\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} c_n e^{-in\omega t} |n\rangle
\]

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where
\[ E_n = \hbar \omega (n + 1/2) \quad , \quad c_n = e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}} \]

We then have
\[
|\psi(t)\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-|\alpha|^2/2} \frac{(ae^{-i\omega t})^n}{\sqrt{n!}} |n\rangle
\]
\[
= e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-|\alpha(t)|^2/2} \frac{(\alpha(t))^{n}}{\sqrt{n!}} |n\rangle
\]

where \( \alpha(t) = \alpha e^{-i\omega t} \). Finally, we have
\[
|\psi(t)\rangle = e^{-i\omega t/2} |\alpha(t)\rangle
\]

At every time, the state is a coherent state with eigenvalue that evolves in time as the classical complex variable.

(ii) 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.

At later times
\[
\langle \psi(t) | \hat{x} | \psi(t) \rangle = \langle \alpha(t) | \hat{x} | \alpha(t) \rangle = x_c Re(\alpha(t)) = x_c Re(\alpha e^{-i\omega t})
\]
\[
\langle \psi(t) | \hat{p} | \psi(t) \rangle = \langle \alpha(t) | \hat{p} | \alpha(t) \rangle = p_c Im(\alpha(t)) = p_c Im(\alpha e^{-i\omega t})
\]

which are the classical equations of motion.

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

The wave function is
\[
\psi_\alpha(t)(x, t) = e^{ip(t)x/\hbar} u_0(x - x(t))
\]
where \( x(t) \) and \( p(t) \) are the classical trajectories. This is an oscillating wave packet, i.e., a gaussian oscillating like a classical SHO.
(j) Show that in the classical limit
\[
\lim_{|\alpha|\to\infty} \frac{\Delta N}{\langle \hat{N} \rangle} \to 0
\]
\[
\langle \hat{N} \rangle = \langle \alpha | \hat{a}^+ \hat{a} | \alpha \rangle = \alpha^* \alpha = |\alpha|^2
\]
\[
\Delta N = \sqrt{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2}
\]
\[
\sqrt{\langle \hat{N}^2 \rangle} = \langle \alpha | (\hat{a}^+ \hat{a})^2 | \alpha \rangle = \langle \alpha | (\hat{a}^+ \hat{a})(\hat{a}^+ \hat{a}) | \alpha \rangle
\]
\[
= \langle \alpha | (\hat{a}^+)^2(\hat{a})^2 | \alpha \rangle + \langle \alpha | \hat{a}^+ [\hat{a}, \hat{a}^+] \hat{a} | \alpha \rangle
\]
\[
= (\alpha^*)^2(\alpha \alpha) + (\alpha^*)(\alpha \alpha) = |\alpha|^4 + |\alpha|^2
\]
Now
\[
\Delta N = \sqrt{|\alpha|^4 + |\alpha|^2 - |\alpha|^4} = \sqrt{|\alpha|^2} = |\alpha|
\]
Therefore, \( \Delta N = \sqrt{\langle \hat{N} \rangle} \) and we have
\[
\lim_{|\alpha|\to\infty} \frac{\Delta N}{\langle \hat{N} \rangle} = \lim_{|\alpha|\to\infty} \frac{1}{\sqrt{\langle \hat{N} \rangle}} \lim_{|\alpha|\to\infty} \frac{1}{|\alpha|} = 0
\]
i.e., the fractional uncertainty goes to zero as the mean amplitude \( \to \) zero.

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

The probability for finding the particle in the \( n^{th} \) excited state is given by
\[
P_n = |\langle n | \alpha \rangle|^2 = |c_n|^2 = |e^{-|\alpha|^2/2} \alpha^n / \sqrt{n!}|^2 = e^{-|\alpha|^2} \frac{|\alpha|^2}{\sqrt{n!}}
\]
Earlier we found that \( \langle n \rangle = |\alpha|^2 \) which gives
\[
P_n = e^{-\langle n \rangle} \frac{(\langle n \rangle)^n}{\sqrt{n!}}
\]
which is the standard Poisson distribution.
(l) Use a *rough* time-energy uncertainty principle ($\Delta E \Delta t > \hbar$), to find an uncertainty principle between the number and phase of a quantum oscillator.

For the oscillator $E \sim n \hbar \omega$ which implies that

$$Et \sim n \hbar (\omega t)$$

Now the phase of the oscillator is $\phi = \omega t$ which then gives

$$\Delta n \Delta \phi \geq 1$$

This is the *number-phase* uncertainty. A quantum oscillator with definite $n$, has uncertain phase!

**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 $\nu_e$, $\nu_\mu$, and $\nu_\tau$. 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

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

and

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

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

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

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 \textit{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.

We will do this problem in two equivalent ways, (1) differential equation method and (2) linear algebraic method.

We have

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \begin{pmatrix} M_0 & 0 & 0 \\ 0 & M_0 & 0 \\ 0 & 0 & M_0 \end{pmatrix} + \begin{pmatrix} 0 & \hbar \omega_1 & \hbar \omega_1 \\ \hbar \omega_1 & 0 & \hbar \omega_1 \\ \hbar \omega_1 & \hbar \omega_1 & 0 \end{pmatrix} = \begin{pmatrix} M_0 & \hbar \omega_1 & \hbar \omega_1 \\ \hbar \omega_1 & M_0 & \hbar \omega_1 \\ \hbar \omega_1 & \hbar \omega_1 & M_0 \end{pmatrix}$$

\textbf{differential equation method:} The Schrodinger equation is

$$\frac{i}{\hbar} \frac{\partial \psi}{\partial t} + \hat{H} \psi = 0$$

where

$$\psi = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = a_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + a_3 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = a_1 |\nu_1\rangle + a_2 |\nu_2\rangle + a_3 |\nu_3\rangle$$

and

$$|\nu_1\rangle = |\nu_e\rangle, \quad |\nu_2\rangle = |\nu_\mu\rangle, \quad |\nu_3\rangle = |\nu_\tau\rangle$$

are basis states and

$$a_i = \text{probability amplitude to have } |\nu_i\rangle$$

This gives the matrix equation

$$i\hbar \begin{pmatrix} \dot{a}_1 \\ \dot{a}_2 \\ \dot{a}_3 \end{pmatrix} = \begin{pmatrix} M_0 & \hbar \omega_1 & \hbar \omega_1 \\ \hbar \omega_1 & M_0 & \hbar \omega_1 \\ \hbar \omega_1 & \hbar \omega_1 & M_0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$
(a) Let $\omega_1 = 0$. then we have

$$a_1(t) = e^{-iM_0 t/\hbar} a_1(0)$$
$$a_2(t) = e^{-iM_0 t/\hbar} a_2(0)$$
$$a_3(t) = e^{-iM_0 t/\hbar} a_3(0)$$

or

$$
\begin{pmatrix}
a_1(t) \\
a_2(t) \\
a_3(t)
\end{pmatrix}
= \hat{U}(t)
\begin{pmatrix}
a_1(0) \\
a_2(0) \\
a_3(0)
\end{pmatrix}
= e^{-iM_0 t/\hbar}
\begin{pmatrix}
a_1(0) \\
a_2(0) \\
a_3(0)
\end{pmatrix}
$$

If the neutrino is initially in one of the basis states, say, $|\nu_1\rangle$, then

$$
\begin{pmatrix}
a_1(0) \\
a_2(0) \\
a_3(0)
\end{pmatrix}
= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
\rightarrow
\begin{pmatrix}
a_1(t) \\
a_2(t) \\
a_3(t)
\end{pmatrix}
= e^{-iM_0 t/\hbar}
\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
= |\nu_1\rangle
$$

or the neutrino stays in the state $|\nu_1\rangle$ or we do not have any oscillations between basis states. The same is true for the other cases.

(b) Let $\omega_1 \neq 0$. Again we assume the neutrino is initially in one of the basis states, say, $|\nu_1\rangle$. Then we have the equations

$$i\hbar \dot{a}_1 = M_0 a_1 + i\omega_1 a_2 + \omega_1 a_3$$
$$i\hbar \dot{a}_2 = M_0 a_2 + i\omega_1 a_1 + \omega_1 a_3$$
$$i\hbar \dot{a}_3 = M_0 a_3 + i\omega_1 a_1 + \omega_1 a_2$$

with boundary conditions

$$a_1(0) = 1 , \quad a_2(0) = 0 , \quad a_3(0) = 0$$

Let

$$a_1(t) = e^{-iM_0 t/\hbar} b_1(t) \rightarrow b_1(0) = 1$$
$$a_2(t) = e^{-iM_0 t/\hbar} b_2(t) \rightarrow b_2(0) = 0$$
$$a_3(t) = e^{-iM_0 t/\hbar} b_3(t) \rightarrow b_3(0) = 0$$

so that we get the new equations

$$\dot{b}_1 = -i\omega_1 (b_2 + b_3)$$
$$\dot{b}_2 = -i\omega_1 (b_1 + b_3)$$
$$\dot{b}_3 = -i\omega_1 (b_1 + b_2)$$

Since there is no way to distinguish $b_2(t)$ and $b_3(t)$ in these equations we must have $b_2(t) = b_3(t)$ in this model., which gives the new equations

$$\dot{b}_1 = -2i\omega_1 b_2$$
$$\dot{b}_2 = -i\omega_1 b_2 - i\omega_1 b_1$$

These give

$$\ddot{b}_2 = -i\omega_1 b_2 - i\omega_1 \dot{b}_1 = -i\omega_1 b_2 - 2\omega_1^2 b_2$$
$$\dot{b}_2 + i\omega_1 b_2 + 2\omega_1^2 b_2 = 0$$

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We assume the solution \( b_2(t) = e^{i\alpha t} \). Substitution converts the differential equation into an algebraic equation for the allowed values of \( \alpha \).

\[
-\alpha^2 + \omega_1 \alpha + 2\omega_1^2 = 0 \rightarrow \alpha = -2\omega_1, +\omega_1
\]

Therefore, the most general solution is

\[
b_2(t) = Ae^{i\omega_1 t} + Be^{-2i\omega_1 t}
\]

Now,

\[
b_2(0) = A + B = 0 \rightarrow B = -A
\]

so that

\[
b_2(t) = A(e^{i\omega_1 t} - e^{-2i\omega_1 t}) = b_3(t)
\]

Returning to the equation for \( b_1(t) \), we then have

\[
b_1 = -2i\omega_1 b_2 = -2i\omega_1 A(e^{i\omega_1 t} - e^{-2i\omega_1 t})
\]

so that

\[
b_1(t) = -2i\omega_1 A \left( \frac{1}{i\omega_1} e^{i\omega_1 t} + \frac{1}{2i\omega_1} e^{-2i\omega_1 t} \right) = -2A \left( e^{i\omega_1 t} + \frac{1}{2} e^{-2i\omega_1 t} \right)
\]

Now

\[
b_1(0) = -3A = 1 \rightarrow A = -\frac{1}{3}
\]

so that

\[
b_1(t) = \frac{2}{3} (e^{i\omega_1 t} + \frac{1}{2} e^{-2i\omega_1 t})
\]

\[
b_2(t) = -\frac{2}{3} (e^{i\omega_1 t} - e^{-2i\omega_1 t}) = b_3(t)
\]

Finally,

\[
P(\nu_e \rightarrow \nu_{\mu}; t) = |a_2(t)|^2 = |b_2(t)|^2 = \left| -\frac{2}{3} (e^{i\omega_1 t} - e^{-2i\omega_1 t}) \right|^2
\]

\[
= \frac{1}{9} \left| e^{i\omega_1 t} - e^{-2i\omega_1 t} \right|^2 = \frac{1}{9} (2 - 2 \cos 3\omega_1 t) = \frac{2}{9} (1 - \cos 3\omega_1 t)
\]

(c) The time of flight of the \( \nu_e \) is \( \Delta t = \ell/v \) in laboratory time. Therefore, the proper time is

\[
\Delta \tau = \frac{\Delta t}{\gamma} = \Delta t \sqrt{1 - \frac{v^2}{c^2}} \approx \frac{\ell M_0}{c E}
\]

where \( E = \) the total energy of the \( \nu_e \) in the rest frame.

For \( P(\nu_e \rightarrow \nu_{\mu}; t) \geq 0.01 \) or

\[
\frac{2}{9} (1 - \cos 3\omega_1 \Delta \tau) \geq 0.01
\]

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we require that

\[
1 - \cos 3\omega_1 \Delta \tau \geq 0.045 \\
0.955 \geq \cos 3\omega_1 \Delta \tau \approx 1 - \frac{9}{2} (\omega_1 \Delta \tau)^2 \\
\omega_1 \geq \frac{\sqrt{2}}{3} \sqrt{0.045} \frac{e^F}{\ell_{SM0}} \approx 0.1 \frac{e^F}{\ell_{SM0}} \\
\hbar \omega_1 \geq 0.05 \text{eV}
\]

**linear algebraic method:** Let us find the eigenvalues and eigenvectors of \( \hat{H} \).

The characteristic equation for the eigenvalues is

\[
\begin{vmatrix}
M_0 - E & h\omega_1 & h\omega_1 \\
h\omega_1 & M_0 - E & h\omega_1 \\
h\omega_1 & h\omega_1 & M_0 - E
\end{vmatrix} = 0 = (M_0 - E)^3 - 3 (M_0 - E) (h\omega_1)^2 + 2 (h\omega_1)^3
\]

or letting \( \alpha = (M_0 - E) \) and \( \beta = h\omega_1 \) we have the equation

\[
\alpha^3 - 3\beta^2 \alpha + 2\beta^3 = 0 \rightarrow \alpha = \beta, \beta, -2\beta
\]

Therefore, the eigenvalues are

\[
E_1 = M_0 + h\omega_1, \ E_2 = E_3 = M_0 - h\omega_1 (2 - \text{fold degeneracy})
\]

Now we obtain the eigenvectors. For \( E_1 = M_0 + h\omega_1 \) we have

\[
\hat{H} |E_1\rangle = E_1 |E_1\rangle = (M_0 + h\omega_1) |E_1\rangle
\]

or

\[
\begin{pmatrix}
M_0 & h\omega_1 & h\omega_1 \\
h\omega_1 & M_0 & h\omega_1 \\
h\omega_1 & h\omega_1 & M_0
\end{pmatrix}
\begin{pmatrix}
a \\
b \\
c
\end{pmatrix}
= (M_0 + h\omega_1)
\begin{pmatrix}
a \\
b \\
c
\end{pmatrix}
\]

or

\[
-2a + b + c = 0 \\
a - 2b + c = 0 \\
a + b - 2c = 0
\]

which imply that

\[
a = b = c = \frac{1}{\sqrt{3}} \text{ (normalized to 1)}
\]

or

\[
|E_1\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}
\]

In a similar manner, for \( E_2 = E_3 = M_0 - h\omega_1 \) we have

\[
|E_2\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}, \quad |E_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}
\]

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Therefore,
\[ |\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \sum_n |E_n\rangle \langle E_n | \psi(0)\rangle = \frac{1}{\sqrt{3}}|E_1\rangle + \frac{1}{\sqrt{6}}|E_2\rangle + \frac{1}{\sqrt{2}}|E_3\rangle \]

Using \( \hat{U}(t) = e^{-i\hat{H}t/\hbar} \), we have
\[ |\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = \sum_n \frac{1}{\sqrt{3}}e^{-iE_1t/\hbar}|E_1\rangle + \frac{1}{\sqrt{6}}e^{-iE_2t/\hbar}|E_2\rangle + \frac{1}{\sqrt{2}}e^{-iE_3t/\hbar}|E_3\rangle \]

Then,
\[ P(\nu_e \rightarrow \nu_\tau; t) = |\langle \nu_\tau | \psi(t)\rangle|^2 \]
where
\[ |\nu_\tau\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \]
or
\[ P(\nu_e \rightarrow \nu_\tau; t) = \frac{1}{3} \left( 1 - \cos \frac{3\omega_1 t}{\hbar} \right) = \frac{2}{9} \left( 1 - \cos \frac{3\omega_1 t}{\hbar} \right) \]
as above.

\textbf{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
\[ N_n = \left( \frac{\alpha}{\sqrt{n!}2^n} \right)^{1/2} = \left( \frac{m\omega}{\hbar} \right)^{1/2} \]

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We have

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

\[ = N_n N_{n'} \int_{-\infty}^{\infty} dx \, H_n(\alpha x) e^{-\frac{1}{2} \alpha^2 x^2} x H_{n'}(\alpha x) e^{-\frac{1}{2} \alpha^2 x^2} \]

\[ = \left( \frac{\alpha}{\sqrt{\pi 2^n n!}} \right)^{1/2} \left( \frac{\alpha}{\sqrt{\pi 2^{n'} n'!}} \right)^{1/2} \int_{-\infty}^{\infty} dx \, e^{-\alpha^2 x^2} x H_n(\alpha x) H_{n'}(\alpha x) \]

Now

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

Therefore let \( q = \alpha x \) and we have

\[ \int_{-\infty}^{\infty} e^{-s^2 + 2sq} e^{-t^2 + 2tq} e^{-q^2} \, dq = \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{s^n t^{n'}}{n! n'!} \int_{-\infty}^{\infty} H_n(q) H_{n'}(q) q e^{-q^2} \, dq \]

or

\[ \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{s^n t^{n'}}{n! n'!} A_{nn'} = \int_{-\infty}^{\infty} e^{-s^2 + 2sq} e^{-t^2 + 2tq} e^{-q^2} \, dq \]

where

\[ A_{nn'} = \int_{-\infty}^{\infty} H_n(\alpha x) H_{n'}(\alpha x) \alpha x e^{-\alpha^2 x^2} \, dx = \frac{1}{N_n N_{n'}} \langle x \rangle_{nn'} \]

Therefore, we are interested in the integral

\[ \int_{-\infty}^{\infty} e^{-s^2 + 2sq} e^{-t^2 + 2tq} e^{-q^2} \, dq = e^{-s^2-t^2} \int_{-\infty}^{\infty} e^{2(s+t)q} e^{-t^2+2tq} e^{-q^2} \, dq \]

\[ = e^{-s^2-t^2} \sqrt{\pi} (s+t) e^{(s+t)^2} = \sqrt{\pi} (s+t) e^{2st} \]

Finally we have

\[ \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{s^n t^{n'}}{n! n'!} A_{nn'} = \int_{-\infty}^{\infty} e^{-s^2 + 2sq} e^{-t^2 + 2tq} e^{-q^2} \, dq \]

\[ = e^{-s^2-t^2} \sqrt{\pi} (s+t) e^{(s+t)^2} = \sqrt{\pi} (s+t) e^{2st} \]

which allows us to determine \( A_{nn'} \) term by term and thus determine \( \langle x \rangle_{nn'} \)
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

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

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

(a) Find the mean position of the particle.

\[
\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) \, dx = \left( \frac{\gamma^2}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} x \exp\left(-\frac{\gamma^2 x^2}{2}\right) \, dx = 0
\]

(b) Find the mean momentum of the particle.

\[
\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hbar \frac{d\psi(x)}{dx} \psi(x) \, dx = -\gamma^2 \hbar \left( \frac{\gamma^2}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} x \exp\left(-\frac{\gamma^2 x^2}{2}\right) \, dx = 0
\]

(c) Find \( V(x) \).

The Schrodinger equation gives

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \rightarrow \frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = (E - V(x)) \psi(x)
\]

\[
-\frac{\hbar^2}{2m} \left(-\gamma^2 + \gamma^4 x^2\right) e^{-\gamma^2 x^2/2} = (E - V(x)) e^{-\gamma^2 x^2/2}
\]

\[
V(x) = E + \frac{\hbar^2}{2m} \left(-\gamma^2 + \gamma^4 x^2\right) = \frac{\hbar^2 \gamma^4}{2m} x^2
\]

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

The Schrodinger equation in the momentum representation is

\[
\left( \frac{p^2}{2m} - \frac{\hbar^4 \gamma^4}{2m} \frac{d^2}{dp^2} \right) \psi(p) = E \psi(p)
\]

which has solution

\[
\psi(p) = Ne^{-\frac{p^2}{2\pi \hbar^2 \gamma^2}}, \quad N = \left( \frac{1}{\pi \hbar^2 \gamma^2} \right)^{1/4}
\]

which is an eigenfunction of the state with energy \( E = \hbar^2 \gamma^2 / 2m \) in the momentum representation.

Therefore,

\[
P(p)dp = |\psi(p)|^2 dp = \left( \frac{1}{\pi \hbar^2 \gamma^2} \right)^{1/2} e^{-\frac{p^2}{2\pi \hbar^2 \gamma^2}} dp
\]
Alternatively, $\psi(p)$ is the Fourier transform of $\psi(x)$, that is,

$$
\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-ipx/\hbar} \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-ipx/\hbar} \left(\frac{\gamma^2}{\pi}\right)^{1/4} \exp \left(-\frac{\gamma^2}{2} x^2/2\right)
$$

$$
= \left(\frac{\gamma^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2\pi\hbar}} \int dx \exp \left(-\frac{p}{\sqrt{2\gamma^2}} - \frac{i\gamma x}{\sqrt{2}}\right) dx = \left(\frac{1}{\pi\gamma^2 \hbar^2}\right)^{1/4} e^{-\frac{p^2}{2\pi\gamma^2}}
$$
as above.

### 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.

Let $|\alpha\rangle = a |0\rangle + b |1\rangle$ where $|a|^2 + |b|^2 = 1$. Then

$$
\langle x \rangle = \langle \alpha | \hat{x} | \alpha \rangle = (a^* \langle 0 | + b^* \langle 1 |) \hat{x} (a |0\rangle + b |1\rangle)
$$

Now we have

$$
\langle m | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1})
$$

Therefore,

$$
\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} (a^* b + b^* a)
$$

Without loss of generality we can choose $a$ and $b$ to be real so that $a^2 + b^2 = 1$ and we have

$$
\langle x \rangle = \sqrt{\frac{2\hbar}{m\omega}} a \sqrt{1 - a^2}
$$

The maximum of $\langle x \rangle$ requires that

$$
\frac{d \langle x \rangle}{da} = 0 \rightarrow a = b = \frac{1}{\sqrt{2}} \rightarrow \langle x \rangle_{\text{max}} = \sqrt{\frac{\hbar}{2m\omega}}
$$

and

$$
|\alpha\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)
$$

(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.
Now

$$|\alpha(t)\rangle = \hat{U}(t) |\alpha\rangle = e^{-i\hat{H}t/\hbar} |\alpha\rangle = \frac{1}{\sqrt{2}} \left( e^{-i\omega t/2\hbar} |0\rangle + e^{-i3\omega t/2\hbar} |1\rangle \right)$$

**Schrodinger Picture:**

$$\langle x(t) \rangle = \langle \alpha(t) | \hat{x} | \alpha(t) \rangle = \frac{1}{2} \left( e^{i\omega t/2\hbar} \langle 0 | + e^{i3\omega t/2\hbar} \langle 1 | \right) \hat{x} \left( e^{-i\omega t/2\hbar} |0\rangle + e^{-i3\omega t/2\hbar} |1\rangle \right)$$

$$= \frac{\hbar}{2m\omega} \frac{1}{2} \left( e^{-i\omega t/\hbar} |0\rangle + e^{i\omega t/\hbar} |1\rangle \right) e^{-i\omega t/\hbar} + e^{i\omega t/\hbar} = \sqrt{\frac{\hbar}{2m\omega}} \cos \omega t$$

**Heisenberg Picture:**

$$\langle x(t) \rangle = \langle \alpha | \hat{x}(t) | \alpha \rangle = \langle \alpha | \hat{x} \cos \omega t + \frac{\hat{p}}{m\omega} \sin \omega t | \alpha \rangle$$

$$= \frac{1}{2} \left( \cos \omega t \left( \langle 0 | \hat{x} | 1 \rangle + \langle 1 | \hat{x} | 0 \rangle \right) + \frac{1}{m\omega} \sin \omega t \left( \langle 0 | \hat{p} | 1 \rangle + \langle 1 | \hat{p} | 0 \rangle \right) \right)$$

$$= \frac{1}{2} \left( \cos \omega t \left( \sqrt{\frac{\hbar}{2m\omega}} + \sqrt{\frac{\hbar}{2m\omega}} \right) + \frac{1}{m\omega} \sin \omega t \left( -\sqrt{\frac{\hbar m\omega}{2}} + \sqrt{\frac{\hbar m\omega}{2}} \right) \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \cos \omega t$$

which is the same for both pictures as expected.

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

Now using the Heisenberg picture we have

$$\langle (\Delta x)^2 \rangle_t = \langle x^2 \rangle_t - \langle x \rangle_t^2 = \langle \alpha | \hat{x}^2(t) | \alpha \rangle - \langle \alpha | \hat{x}(t) | \alpha \rangle^2$$

From (b) we have

$$\langle \alpha | \hat{x}(t) | \alpha \rangle = \sqrt{\frac{\hbar}{2m\omega}} \cos \omega t$$

The other term becomes

$$\langle \alpha | \hat{x}^2(t) | \alpha \rangle = \frac{\hbar}{2m\omega} \left( \langle 0 | + \langle 1 | \right) \left( e^{i\hat{H}t/\hbar} (\hat{a} + \hat{a}^+)^2 e^{-i\hat{H}t/\hbar} \right) (\langle 0 | + \langle 1 |)$$

$$= \frac{\hbar}{2m\omega} \left( \langle 0 | + \langle 1 | \right) \left( \hat{a} e^{-2i\omega t} + \hat{a} \hat{a} e^{-2i\omega t} + \hat{a} \hat{a}^+ e^{2i\omega t} + \hat{a}^+ \hat{a}^+ e^{2i\omega t} \right) (\langle 0 | + \langle 1 |)$$

$$= \frac{\hbar}{2m\omega} \left( \langle 1 | \hat{a} \hat{a}^+ | 0 \rangle + \langle 0 | \hat{a}^+ \hat{a} | 1 \rangle \right) = \frac{\hbar}{2m\omega}$$

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Therefore,
\[ \langle (\Delta x)^2 \rangle_t = \frac{\hbar}{2m\omega} (1 - \cos^2 \omega t) = \frac{\hbar}{2m\omega} \sin^2 \omega t \]

### 8.15.27 Coupled oscillators

Two identical harmonic oscillators in one dimension each have a mass \( m \) and frequency \( \omega \). 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.

We have
\[
\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{\text{int}} = \frac{\hat{p}_1^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}_2^2 + C\hat{x}_1 \hat{x}_2
\]

We shift to CM coordinates
\[
\hat{X} = \frac{\hat{x}_1 - \hat{x}_2}{2}, \quad \hat{Y} = \frac{\hat{x}_1 + \hat{x}_2}{2}
\]
\[
\hat{P} = \frac{\hat{p}_1 - \hat{p}_2}{2}, \quad \hat{\phi} = \hat{p}_1 + \hat{p}_2
\]
or
\[
\hat{x}_1 = \frac{\hat{X}}{2} + \hat{Y}, \quad \hat{x}_2 = -\frac{\hat{X}}{2} + \hat{Y}
\]
\[
\hat{p}_1 = \hat{P} + \frac{\hat{\phi}}{2}, \quad \hat{p}_2 = -\hat{P} + \frac{\hat{\phi}}{2}
\]
which gives
\[
\hat{H} = \left[ \frac{\hat{P}^2}{m} + \frac{mX^2}{4} \left( \omega^2 - \frac{C}{m} \right) \right] + \left[ \frac{\hat{\phi}^2}{4m} + mY^2 \left( \omega^2 + \frac{C}{m} \right) \right]
\]
which represents two uncoupled oscillators.

The X-oscillator has frequency \( \Omega_X = \sqrt{\omega^2 - C/m} \) and energy eigenvalues \( E_{n_X}^X = \hbar\Omega_X (n_X + 1/2) \), \( n_X = 0, 1, 2, ... \).

The Y-oscillator has frequency \( \Omega_Y = \sqrt{\omega^2 + C/m} \) and energy eigenvalues \( E_{n_Y}^Y = \hbar\Omega_Y (n_Y + 1/2) \), \( n_Y = 0, 1, 2, ... \).

Therefore,
\[
E_{n_Xn_Y} = E_{n_X}^X + E_{n_Y}^Y = \hbar\Omega_X (n_X + 1/2) + \hbar\Omega_Y (n_Y + 1/2)
\]

### 8.15.28 Interesting operators ....

The operator \( \hat{c} \) is defined by the following relations:
\[
\hat{c}^2 = 0, \quad \hat{c}\hat{c}^+ + \hat{c}^+\hat{c} = \{\hat{c}, \hat{c}^+\} = \hat{I}
\]

(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. \( \hat{c}^+ |0\rangle = |1\rangle \), \( \hat{c} |0\rangle = 0 \)

We define

\[ \hat{c}^2 = 0 \quad \text{and} \quad \hat{c} \hat{c}^+ + \hat{c}^+ \hat{c} = \{ \hat{c}, \hat{c}^+ \} = I \]

Then

\[ \hat{N} = \hat{c}^+ \hat{c} \rightarrow \hat{N}^+ = (\hat{c}^+ \hat{c})^+ = \hat{c}^+ \hat{c} = \hat{N} \rightarrow \text{Hermitian} \]
\[ \hat{N}^2 = \hat{c}^+ \hat{c} \hat{c}^+ \hat{c} = \hat{c}^+ (I - \hat{c}^+ \hat{c}) \hat{c} = \hat{c}^+ \hat{c} = \hat{N} \]

Therefore,

\[ \hat{N} |\lambda\rangle = \lambda |\lambda\rangle \rightarrow (\hat{N}^2 - \hat{N}) |\lambda\rangle = (\lambda^2 - \lambda) |\lambda\rangle = 0 \rightarrow \lambda = 0, 1 \]

such that
\[
\begin{align*}
\hat{N} |1\rangle &= |1\rangle \rightarrow \hat{c}^+ \hat{c} |1\rangle = |1\rangle \rightarrow (I - \hat{c}^+ \hat{c}) |1\rangle = |1\rangle \rightarrow \hat{c} \hat{c}^+ |1\rangle = 0 \\
\hat{N} |0\rangle &= 0 \rightarrow \hat{c}^+ \hat{c} |0\rangle = 0 \rightarrow (I - \hat{c}^+ \hat{c}) |0\rangle = 0 \rightarrow \hat{c} \hat{c}^+ |0\rangle = |0\rangle 
\end{align*}
\]

We then have
\[
\begin{align*}
\langle 1 | \hat{c} \hat{c}^+ |1\rangle &= 0 = \| \hat{c}^+ |1\rangle \|^2 \rightarrow \hat{c}^+ |1\rangle = 0 \\
\langle 0 | \hat{c} \hat{c}^+ |0\rangle &= 0 = \| \hat{c} |0\rangle \|^2 \rightarrow \hat{c} |0\rangle = 0 
\end{align*}
\]

Now
\[ \langle 0 | \hat{c} \hat{c}^+ |0\rangle = \langle 0 | 0 \rangle = 1 \rightarrow \| \hat{c}^+ |0\rangle \|^2 = 1 \]

If we suppose that
\[
\begin{align*}
\hat{c}^+ |0\rangle &= a |0\rangle + b |1\rangle \\
\hat{c} \hat{c}^+ |0\rangle &= 0 = a \hat{c}^+ |0\rangle + b \hat{c}^+ |1\rangle = a \hat{c}^+ |0\rangle 
\end{align*}
\]

which says that either \( \hat{c}^+ |0\rangle = 0 \) (inconsistent with earlier result) or \( a = 0 \).

Therefore, \( \hat{c}^+ |0\rangle = |1\rangle \) (\( b = 1 \) for consistency).

Finally, we have
\[
\begin{align*}
\langle 1 | \hat{c} \hat{c}^+ |1\rangle &= \langle 1 | 1 \rangle = 1 \rightarrow \| \hat{c} |1\rangle \|^2 = 1 \\
\langle 0 | \hat{c} \hat{c}^+ |0\rangle &= \langle 0 | 0 \rangle = 1 \rightarrow \| \hat{c} |0\rangle \|^2 = 1 
\end{align*}
\]

If we suppose that
\[
\begin{align*}
\hat{c} |1\rangle &= a |1\rangle + b |0\rangle \\
\hat{c} \hat{c} |1\rangle &= 0 = a \hat{c} |1\rangle + b \hat{c} |0\rangle = a \hat{c} |1\rangle 
\end{align*}
\]

which says that either \( \hat{c} |1\rangle = 0 \) (inconsistent with earlier result) or \( b = 0 \).

Therefore, \( \hat{c} |1\rangle = |0\rangle \) (\( a = 1 \) for consistency).

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(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).

Let
\[ \hat{H} = \hbar \omega_0 (\hat{c}^+ \hat{c} + 1/2) , \hat{H} |n\rangle = E_n |n\rangle \]

and assume that
\[ |n\rangle = a_n |0\rangle + b_n |1\rangle \]

We then have
\[ \hat{H} |n\rangle = \hbar \omega_0 (\hat{c}^+ \hat{c} + 1/2) (a_n |0\rangle + b_n |1\rangle) = \hbar \omega_0 b_n |1\rangle + \frac{\hbar \omega_0}{2} |n\rangle \]

Cases:
\[ n = 0 \rightarrow a_0 = 1 , b_0 = 0 \rightarrow E_0 = \frac{\hbar \omega_0}{2} \]
\[ n = 1 \rightarrow a_1 = 0 , b_1 = 1 \rightarrow E_1 = \frac{3\hbar \omega_0}{2} \]

No other choices of \((a_n, b_n)\) pairs work (satisfy the eigenvector/eigenvalue equation)!

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

These operators are describing fermions where we can only have 0 or 1 particle in any state.

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 \( t \)?

We have
\[ |\psi(0)\rangle = a |0\rangle + b |1\rangle \]
\[ P(E = \hbar \omega/2) = |a|^2 = \frac{1}{2} \rightarrow a = \frac{1}{\sqrt{2}} \]
\[ P(E = 3\hbar \omega/2) = |b|^2 = \frac{1}{2} \rightarrow b = \frac{1}{\sqrt{2}} e^{i\alpha} \]

so that
\[ |\psi(0)\rangle = \frac{1}{\sqrt{2}} (|0\rangle + e^{i\alpha} |1\rangle) \]

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Now
\[ \langle p \rangle_{t=0} = \langle \psi(0) | \hat{p} | \psi(0) \rangle = \sqrt{\frac{m\omega\hbar}{2}} \]
\[ = \frac{i}{2} \sqrt{\frac{m\omega\hbar}{2}} \left( \langle 0 | + e^{-i\alpha} \langle 1 | (\hat{a}^+ - \hat{a}) \langle 0 | + e^{i\alpha} | 1 \rangle \right) \]
\[ = \frac{i}{2} \sqrt{\frac{m\omega\hbar}{2}} \left( -e^{i\alpha} \langle 0 | \hat{a} | 1 \rangle + e^{-i\alpha} \langle 1 | \hat{a}^+ | 0 \rangle \right) \]
\[ = \frac{i}{2} \sqrt{\frac{m\omega\hbar}{2}} (-e^{i\alpha} + e^{-i\alpha}) = \sin \alpha \sqrt{\frac{m\omega\hbar}{2}} \]
so that
\[ \sin \alpha = 1 \rightarrow \alpha = \frac{\pi}{2} \]
and
\[ | \psi(0) \rangle = \frac{1}{\sqrt{2}} \left( | 0 \rangle + e^{i\frac{\pi}{2}} | 1 \rangle \right) = \frac{1}{\sqrt{2}} \left( | 0 \rangle + i | 1 \rangle \right) \]
Then we have
\[ | \psi(t) \rangle = \frac{1}{\sqrt{2}} \left( e^{-i\omega t/2} | 0 \rangle + ie^{-3i\omega t/2} | 1 \rangle \right) \]
and
\[ \langle p \rangle_{t} = \langle \psi(t) | \hat{p} | \psi(t) \rangle \]
\[ = \frac{i}{2} \sqrt{\frac{m\omega\hbar}{2}} \left( e^{i\omega t/2} \langle 0 | - ie^{3i\omega t/2} \langle 1 | (\hat{a}^- + \hat{a}) \left( e^{-i\omega t/2} | 0 \rangle + ie^{-3i\omega t/2} | 1 \rangle \right) \right) \]
\[ = \frac{i}{2} \sqrt{\frac{m\omega\hbar}{2}} \left( -ie^{i\omega t} \langle 0 | \hat{a} | 1 \rangle - ie^{-i\omega t} \langle 1 | \hat{a}^+ | 0 \rangle \right) \]
\[ = \frac{1}{2} \sqrt{\frac{m\omega\hbar}{2}} \left( e^{-i\omega t} + e^{i\omega t} \right) = \sqrt{\frac{m\omega\hbar}{2}} \cos \omega t \]

8.15.30 Things about particles in box

A particle of mass m moves in a one-dimensional box (Infinite well) of length \( \ell \) 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
\[ \psi(x, 0) = \begin{cases} \sqrt{\frac{30}{\ell^5}} x (\ell - x) & 0 < x < \ell \\ 0 & \text{otherwise} \end{cases} \]
(a) Write this wave function as a linear combination of energy eigenfunctions

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

We have

\[ \psi(x, 0) = \sum_{n} a_n \psi_n(x) \]

which gives

\[ \int \psi_k^*(x) \psi(x, 0) \, dx = \sum_{n} a_n \int \psi_k^*(x) \psi_n(x) \, dx = \sum_{n} a_n \delta_{nk} = a_k \]

Therefore

\[ a_k = \sqrt{\frac{60}{\ell^6}} \int_{0}^{\ell} x(\ell - x) \sin \frac{\pi k x}{\ell} \, dx \]

\[ = \sqrt{\frac{60}{\ell^6} \ell^3} \frac{\pi^3}{k^3\pi^3} (2 - \cos k\pi + k\pi \sin k\pi) \]

\[ = \frac{8\sqrt{15}}{k^3\pi^3} k = 1, 3, 5, \ldots \]

and \( a_k = 0 \) for \( k = 2, 4, \ldots \).

Therefore,

\[ \psi(x, 0) = \sum_{m \text{ odd}} \frac{8\sqrt{15}}{m^3\pi^3} \psi_m(x) \]

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

\[ P(E_n) = |a_n|^2 = \begin{cases} \frac{960}{m^6\pi^6} & m = 1, 3, 5, \ldots \\ 0 & \text{otherwise} \end{cases} \]

NOTE: Since

\[ \sum_{n} P(E_n) = 1 \]

we have

\[ \frac{960}{\pi^6} \sum_{n \text{ odd}} \frac{1}{n^6} = 1 \rightarrow \sum_{n \text{ odd}} \frac{1}{n^6} = \frac{\pi^6}{960} = 1.00145 \]

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

\[ \psi(x, t > 0) = \sum_{m \text{ odd}} a_m \psi_m(x) e^{-iE_m t/\hbar} \]

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:
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 $\vec{E}$, which alters the potential energy as shown in the figure below:

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

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

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.

We have

$$T \approx \exp \left( -2 \int \sqrt{\frac{2m}{\hbar^2}} \sqrt{V(x) - Edx} \right)$$

where

$$(W + E_f) - e\varepsilon x = V(x) \quad \text{(assumes barrier maximum at x = 0)}$$
At \( x = L \), we have

\[
(W + E_f) - e\varepsilon L = E_f \rightarrow W = e\varepsilon L
\]

Therefore,

\[
T \approx \exp \left(-2 \int_0^L \sqrt{\frac{2m}{\hbar^2}} \sqrt{(W + E_f) - e\varepsilon x - E_f} \, dx \right)
\]

\[
= \exp \left(-\sqrt{\frac{8m}{\hbar^2}} \int_0^L \sqrt{W - e\varepsilon x} \, dx \right)
\]

\[
= \exp \left(-\sqrt{\frac{8me\varepsilon}{\hbar^2}} \int_0^L \sqrt{L - x} \, dx \right) = \exp \left(-\frac{4}{3} \sqrt{\frac{2m}{\hbar^2}} W^{3/2} \varepsilon \right)
\]

**Approximating an Arbitrary Barrier**

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

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

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

\[
\sinh \gamma a = \frac{e^{\gamma a} - e^{-\gamma a}}{2} \to e^{\gamma a}
\]

so that

\[
T = \frac{1}{1 + \left(\frac{\gamma^2 + k^2}{4k\gamma}\right)^2 \sinh^2 \gamma a} \to 1 + \left(\frac{4k\gamma}{\gamma^2 + k^2}\right)^2 e^{-2\gamma a}
\]

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

\[
\ln T \to \ln \left(\frac{4k\gamma}{\gamma^2 + k^2}\right)^2 - 2\gamma a \to -2\gamma a
\]

where we have dropped the logarithm relative to \( \gamma a \) since \( \ln(\text{almost anything}) \) 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:
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 $\Delta x$) 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 $m = 0.8 \times 10^{-24} \text{ gm}$ in the well shown in the figure below:
The size of the well (range of the potential) is $a = 1.4 \times 10^{-13} \text{ cm}$. If the binding energy of the system is $2.2 \text{ MeV}$, find the depth of the potential $V_0$ in $\text{ MeV}$.

This is a model of the deuteron in one dimension.

We have two regions to consider. We let $E = -|E|$. For $0 \leq x \leq a$

$$
\psi_I(x) = Ae^{ikx} + Be^{-ikx}, \quad \frac{\hbar^2 k^2}{2m} = V_0 - |E|
$$

For $x \geq a$

$$
\psi_{II}(x) = Ce^{-\gamma x}, \quad \frac{\hbar^2 \gamma^2}{2m} = |E|
$$

We now impose boundary conditions at $x = 0$ and $x = a$:

- $\psi_I(0) = 0 \rightarrow A = -B \rightarrow \psi_I(x) = A \sin kx$
- $\psi_I(a) = \psi_{II}(a) \rightarrow A \sin ka = C e^{-\gamma a}$
- $\psi_I'(a) = \psi_{II}'(a) \rightarrow kA \cos ka = -\gamma Ce^{-\gamma a}$

These give

$$
\tan ka = -\frac{k}{\gamma} \rightarrow \tan \left(\frac{2m |E|}{\hbar^2} a^2\right)^{1/2} \left(\frac{V_0}{|E|} - 1\right)^{1/2} = -\left(\frac{V_0}{|E|} - 1\right)^{1/2}
$$

Now,

$$
\left(\frac{2m |E|}{\hbar^2} a^2\right)^{1/2} = \left(\frac{2(0.8 \times 10^{-27})(2.2 \times 10^6 \times 1.6 \times 10^{-19})}{(1.05 \times 10^{-34})^2}(1.4 \times 10^{-15})^2\right)^{1/2} = 0.32
$$

Therefore, we have

$$
\tan 0.32 \left(\frac{V_0}{|E|} - 1\right)^{1/2} = -\left(\frac{V_0}{|E|} - 1\right)^{1/2}
$$

This is solved by

$$
\left(\frac{V_0}{|E|} - 1\right)^{1/2} \approx 5.5 \rightarrow V_0 = 31.25 |E| = 66.55 \text{ MeV}
$$
8.15.33 Use Matrix Methods

A one-dimensional potential barrier is shown in the figure below.

Figure 8.10: A Potential Barrier

Define and calculate the transmission probability for a particle of mass $m$ and 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.

We have three regions to consider:

(I) $x \leq 0$ \hspace{0.5cm} $E = \frac{\hbar^2 k^2}{2m}$ \hspace{0.5cm} $\psi_I(x) = e^{ikx} + Re^{-ikx}$

(II) $0 \leq x \leq a$ \hspace{0.5cm} $V_0 - E = \frac{\hbar^2 \alpha^2}{2m}$ \hspace{0.5cm} $\psi_{II}(x) = Ae^{-\alpha x} + Be^{\alpha x}$

(III) $x \geq a$ \hspace{0.5cm} $E - V_1 = \frac{\hbar^2 k'^2}{2m}$ \hspace{0.5cm} $\psi_{III}(x) = Te^{ikx}$

Boundary conditions:

\[
\psi_I(0) = \psi_{II}(0) \to 1 + R = A + B \\
\psi_{II}(a) = \psi_{III}(a) \to Ae^{-\alpha a} + Be^{\alpha a} = Te^{ik'a} \\
\frac{d}{dx}\psi_I(0) = \frac{d}{dx}\psi_{II}(0) \to ik(1 - R) = -\alpha(A - B) \\
\frac{d}{dx}\psi_{II}(a) = \frac{d}{dx}\psi_{III}(a) \to -\alpha(Ae^{-\alpha a} - Be^{\alpha a}) = ik'Te^{ik'a}
\]

Written in matrix form these equations are:

\[
\begin{pmatrix}
1 & 1 \\
-ik & -ik
\end{pmatrix}
\begin{pmatrix}
1 \\
R
\end{pmatrix}
= 
\begin{pmatrix}
1 & 1 \\
-\alpha & \alpha
\end{pmatrix}
\begin{pmatrix}
A \\
B
\end{pmatrix}
\]

\[
\begin{pmatrix}
e^{-\alpha a} & e^{\alpha a} \\
-\alpha e^{-\alpha a} & \alpha e^{\alpha a}
\end{pmatrix}
\begin{pmatrix}
A \\
B
\end{pmatrix}
= 
\begin{pmatrix}
1 \\
(ik')
\end{pmatrix}
Te^{ik'a}
\]

or

\[
\begin{pmatrix}
1 \\
R
\end{pmatrix}
= 
\begin{pmatrix}
1 & 1 \\
-ik & -ik
\end{pmatrix}^{-1}
\begin{pmatrix}
1 & 1 \\
-\alpha & \alpha
\end{pmatrix}^{-1}
\begin{pmatrix}
e^{-\alpha a} & e^{\alpha a} \\
-\alpha e^{-\alpha a} & \alpha e^{\alpha a}
\end{pmatrix}^{-1}
\begin{pmatrix}
1 \\
(ik')
\end{pmatrix}
Te^{ik'a} = M
\begin{pmatrix}
1 \\
(ik')
\end{pmatrix}
Te^{ik'a}
\]

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Therefore we have

\[
M = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 \\ -\alpha & \alpha \end{pmatrix} \begin{pmatrix} e^{-\alpha a} & e^{\alpha a} \\ -\alpha e^{-\alpha a} & \alpha e^{\alpha a} \end{pmatrix}^{-1} \\
\frac{1}{4i\alpha k} \begin{pmatrix} -ik & -1 \\ -ik & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ \alpha e^{\alpha a} & -e^{\alpha a} \end{pmatrix} \\
\frac{1}{4i\alpha k} \left( \alpha \left[ (\alpha - ik) e^{\alpha a} - (\alpha + ik) e^{-\alpha a} \right] \left[ - (\alpha - ik) e^{\alpha a} - (\alpha + ik) e^{-\alpha a} \right] \right) \\
\frac{1}{4i\alpha k} \left( \alpha \left[ -(\alpha + ik) e^{\alpha a} + (\alpha - ik) e^{-\alpha a} \right] \left[ (\alpha + ik) e^{\alpha a} + (\alpha - ik) e^{-\alpha a} \right] \right)
\]

or

\[
1 = \frac{i}{4\alpha k} \left( (\alpha - ik') (\alpha - ik) e^{\alpha a} - (\alpha + ik') (\alpha - ik) e^{-\alpha a} \right) e^{ik'a} T
\]

Rearranging we have

\[
T = \frac{-4i\alpha k e^{-ik'a}}{(\alpha - ik') (\alpha - ik) e^{\alpha a} - (\alpha + ik') (\alpha - ik) e^{-\alpha a}} \\
= \frac{\alpha^2 - kk' e^{\alpha a} - i\alpha (k + k') e^{\alpha a}}{-4i\alpha e^{-ik'a}} \\
= \frac{\left( \frac{\alpha^2}{2} - \frac{k k'}{\alpha} \right) e^{\alpha a} - i \left( 1 + \frac{k k'}{\alpha^2} \right) e^{\alpha a} - \left( \frac{\alpha}{2} + \frac{k k'}{\alpha^2} \right) e^{-\alpha a} + i \left( 1 - \frac{k k'}{\alpha^2} \right) e^{-\alpha a}}{-2ie^{-ik'a}} \\
= \frac{(\frac{\alpha^2}{2} - i) \sinh \alpha a - (i \frac{k k'}{\alpha} + \frac{k k'}{\alpha}) \cosh \alpha a}
\]

The limits \( V_1 \to 0 \), \( k' \to k \), \( a \to 2a \) give the standard result

\[
T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)}} \sinh^2 \alpha a
\]

### 8.15.34 Finite Square Well Encore

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

(a) Let \( k_0 = \sqrt{2mV_0/\hbar^2} \). 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) \( \frac{k_0a}{2} = 5 \)

The finite square well is shown below

![Finite Square Well Diagram](image-url)
In Chapter 8 we showed that the solutions could be found as simultaneous solutions of:

**Even Parity:**

\[ y = +x \tan x, \quad x^2 + y^2 = r^2 \]

**Odd Parity:**

\[ y = -x \cot x, \quad x^2 + y^2 = r^2 \]

where

\[ y = \frac{\kappa a}{2}, \quad x = \frac{ka}{2} \]

\[ \kappa = \sqrt{\frac{2mE_b}{\hbar^2}}, \quad k = \sqrt{\frac{2m(V_0 - E_b)}{\hbar^2}} \]

and \( x, y > 0 \), \( r = k_0a/2 > 0 \). Shown below are the solutions for the three different choices of \( r = k_0a/2 > 0 \).

**Case (i):** \( k_0a/2 = 1 \)

We have one bound state with a wave function as shown below:
Case (ii): $k_0a/2 = 1.6$

We have two bound states with a wave functions as shown below:

![Wave functions for Case (ii)](image)

Case (iii): $k_0a/2 = 5$

We have four bound states with a wave functions as shown below:

![Wave functions for Case (iii)](image)

NOTE: The states deep in the well (i.e., the ground and first excited states) are close to the infinite well solutions.

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

From the graphical solution we see that there is always one solution for $0 < k_0a/2 < \pi/2$. This is an even parity solution as shown below:

![Even parity solution](image)

(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 $E_b = mU_0^2/2\hbar^2$.

We seek the solution to the delta function potential as the limit of our
graphical solution to the finite well.

We take the limit $V_0 \to \infty, a \to 0$ such that $V_0 a \to U_0$, a constant. Thus,

$$k_0 a = \sqrt{\frac{2m}{\hbar^2}} \sqrt{V_0 a} = \sqrt{\frac{2m}{\hbar^2 V_0}} V_0 a = \sqrt{\frac{2m}{\hbar^2}} \frac{U_0}{\sqrt{V_0}} \to 0$$

Thus, we expect one bound state from the argument above and we have

$$\kappa a \to 0, \quad ka \to 0$$

and thus

$$\lim_{\kappa a, ka \to 0} \left( \frac{ka}{2} \tan \left( \frac{ka}{2} \right) = \frac{\kappa a}{2} \right) \to \frac{(ka)^2}{4} = \frac{\kappa a}{2}$$

This implies that

$$\kappa = \frac{k^2 a}{2} = \frac{a}{2} \left( \frac{2m(V_0 - E_b)}{\hbar^2} \right) \to \frac{mU_0}{\hbar^2}$$

since $aV_0 = U_0 \gg aE_b$ in the limit and

$$E_b = \frac{\hbar^2 \kappa^2}{2m} = \frac{mU_0^2}{2\hbar^2}$$

which is the correct energy for the delta potential well.

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

![Figure 8.11: Half-Infinite, Half-Finite Well](image_url)
Without doing any calculation, show that there are no bound states unless \( k_0 L > \pi / 2 \). HINT: think about erecting an infinite wall down the center of a symmetric finite well of width \( a = 2L \). Also, think about parity.

The stationary states of a symmetric finite well of width \( a = 2L \) must satisfy the boundary condition \( \psi(0) = 0 \) (at the center - where the infinite wall is place!). But the odd parity solutions of the well are already zero at the center \( (x = 0) \). Therefore, the odd parity solutions of a well with \( a = 2L \) have the same spectrum as our half-infinite, half-finite well.

The odd parity solutions require
\[
\frac{k_0 a}{2} > \frac{\pi}{2} \rightarrow k_0 L > \frac{\pi}{2} \]

(e) Show that in general, the binding energy eigenvalues satisfy the eigenvalue equation
\[
\kappa = -k \cot kL
\]
where
\[
\kappa = \sqrt{\frac{2mE_b}{\hbar^2}} \quad \text{and} \quad k^2 + \kappa^2 = k_0^2
\]
If we substitute
\[
\frac{ka}{2} = kL
\]
in the odd parity transcendental equation above we get
\[
\kappa = -k \cot kL
\]
as required.

8.15.35 Half-Infinite Half-Finite Square Well Encore

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

![Figure 8.12: Half-Infinite, Half-Finite Well Again](image-url)
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, \( \psi_{\text{in}}(x) = Ae^{-ikx} \), where the particle has energy \( E = (\hbar k)^2 / 2m \), the reflected wave will emerge from the potential with a phase shift, \( \psi_{\text{out}}(x) = Ae^{ikx+\phi} \).

**Warm Up:** Consider a free particle on the half-line with an infinite wall at \( x = 0 \).

General solution to T.I.S.E.:

\[
\psi(x) = Be^{ikx} + Ae^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}
\]

with boundary condition \( \psi(0) = 0 \), which implies that \( B = -A \). This corresponds to a standing wave.

NOTE: The standing wave is a superposition of two traveling waves. The relative phase is fixed by the boundary conditions. The overall complex amplitude is not fixed. Instead it is chosen by the asymptotic conditions:

We have an incident wave from \( x = +\infty \), \( \psi_{\text{inc}} = Be^{ikx} = -Ae^{ikx} \) and the outgoing wave to \( x = +\infty \), \( \psi_{\text{out}} = -Ae^{ikx} \).

We now consider the half-infinite, half-finite well.
(a) Show that the reflected wave is phase shifted by

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

where

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

By conservation of probability

$$J_{inc} = J_{out} \to \frac{hk}{m} |A|^2 = \frac{hk}{m} |B|^2 \to |B| = |A|$$

We will look for solutions of the form

$$B = -A e^{i\phi}$$

This form is chosen so that when \( V_0 = 0 \), then \( \phi = 0 \) as shown previously. These are the asymptotic forms of the full solutions of the problem shown below.

We have

**Region I:**

$$u_I(x) = C \sin (qx), \quad q = \sqrt{\frac{2m(E + V_0)}{\hbar^2}}$$

**Region II:**

$$u_{II}(x) = A e^{-ikx} + B e^{ikx} = A e^{-ikx} - A e^{ikx+i\phi} = -2iAe^{i\phi/2} \sin (kx + \phi/2)$$

Matching boundary conditions:

$$u_I(L) = u_{II}(L) \to C \sin (qL) = -2iAe^{i\phi/2} \sin (kL + \phi/2)$$

$$\frac{du_I(L)}{dx} = \frac{du_{II}(L)}{dx} \to qC \cos (qL) = -2ikAe^{i\phi/2} \cos (kL + \phi/2)$$

Dividing the two equations we get

$$\tan (kL + \phi/2) = \frac{k}{q} \tan (qL)$$
Therefore,

\[ kL + \phi/2 = \tan^{-1}\left( \frac{k}{q} \tan (qL) \right) \]

which implies that

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

(b) Plot the function of \( \phi \) as a function of \( k_0L \) for fixed energy. Comment on your plot.

When plotting \( \phi \), one should remember \( \phi = \phi \mod 2\pi \) since \( \phi \) and \( \phi + 2\pi \) are the same phase.

We consider this as a function of \( k_0L \) for a fixed energy where

\[ k_0 = \sqrt{\frac{2mV_0}{k^2}} \]

Let

\[ \tilde{k} = \frac{k}{k_0} = \sqrt{\frac{E}{V_0}} \text{ take fixed} \]

\[ \frac{q}{k_0} = \left( \frac{E}{V_0} + 1 \right)^{1/2} = (\tilde{k}^2 + 1)^{1/2} \]

Let \( \theta = k_0L \). This then implies that

\[ \phi = 2 \tan^{-1}\left( \frac{\tilde{k}}{\tilde{k}^2 + 1}^{1/2} \tan (\theta(\tilde{k}^2 + 1)^{1/2}) \right) - 2\tilde{k}\theta \]

we want to plot this as a function of \( \theta \) for a fixed \( \tilde{k} \) (i.e., change \( L \)). Shown below is a plot of \( \phi(\theta) \) for \( \tilde{k} = \sqrt{E/V_0} = 0.1 \ll 1 \) which implies that

\[ \phi \approx 2 \tan^{-1}(0.1 \tan (\theta)) - 0.2\theta \]
We see these important features:

The phase shift is a weak function of $\theta$ except when $\theta = n\pi/2 = k_0 L$. At these points the phase jumps by $\pi$.

The jumps occur exactly at the bound states of the well, i.e., every time the well develops a new bound state the phase jumps by $\pi$.

(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 8.13: Shifted Wall](image)

What is the effective $L'$ as a function of the phase shift $\phi$ 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.

Here, we find the phase shift through the boundary condition

$$\psi(L) = \psi_{in}(L) + \psi_{out}(L) = 0 \rightarrow \sin (kL' + \phi/2) = 0$$
We can choose $kL' + \phi/2 = 0$. Therefore, we can achieve the scattering phase shift from the hard wall at $x = L'$ as in the well if we choose

$$L' = -\frac{\phi(k)}{2k}$$

where $\phi(k)$ is given in (b).

**NOTE:**

Positive phase shift $\rightarrow L' < 0$ or wall shifted to the left

Negative phase shift $\rightarrow L' > 0$ or wall shifted to the right

### 8.15.36 Nuclear $\alpha$ Decay

Nuclear alpha–decays $(A, Z) \rightarrow (A - 2, Z - 2) + \alpha$ 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.

![Figure 8.14: Nuclear Potential Model](image-url)
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 \(a = 5\) fm and the kinetic energy of the \(\alpha\) particle 1 MeV, 3 MeV, 10 MeV, 30 MeV.

We compute the integral

\[
V = \frac{2(Z-2)q^2}{r}; \quad tp = \frac{2(Z-2)q^2}{E_0};
\]

\[
\text{Tint}[x_] = \text{Integrate}[\sqrt{2m(V - E_0)} \, x]
\]

\[
\sqrt{2} \left[ \sqrt{m(E_0 - 2q^2 - 2Z/r)} - \frac{2q^2 \sqrt{m(E_0 - 2q^2 - 2Z/r)}}{\sqrt{E_0 \sqrt{4q^2 + 2q^2 + E_0} \sqrt{2q^2 + 2q^2 + E_0}} \sqrt{2q^2 - 2Z/r}} \right]
\]

to give the turning points and probabilities

\[
\text{erytomev} = 624\,150.97;
\]

\[
\text{constants} = \{m \rightarrow 3727.37917 / (2.99792458 \times 10^{10})^2, \quad h \rightarrow 6.59211915 \times 10^{-22}, \quad Z \rightarrow 92, \quad a \rightarrow 5 \times 10^{-12}, \quad q \rightarrow 4.802 \times 10^{-10} \times \sqrt{\text{erytomev}} \};
\]

\[
\text{energies} = \{1, 3, 10, 30\};
\]

\[
\text{T} = \text{Exp}\left[-\frac{2}{\hbar} (\text{Tint}[b] - \text{Tint}[a])\right];
\]

\[
(\text{tp} / \cdot \text{EO} = \text{energies} / \cdot \text{constants}) * 0.01
\]

\[
(\text{T} / \cdot \text{b} \rightarrow \text{tp} = \text{MachineEpsilon}) / \cdot \text{EO} = \text{energies} / \cdot \text{constants} / \cdot \text{Re}
\]

\[
\{2.59064 \times 10^{-12}, 8.63545 \times 10^{-14}, 2.59064 \times 10^{-14}, 8.63545 \times 10^{-15} \}
\]

\[
\{4.09218 \times 10^{-12}, 6.29166 \times 10^{-12}, 3.4055 \times 10^{-22}, 0.000152428 \}
\]
Mathematica note: The integral blows up at the classical turning point $b$, so this must be handled numerically. In the above computation we take $b \rightarrow b - \epsilon$, where $\epsilon$ is the $MachineEpsilon$, or the upper bound of positive numbers $\delta$ for which $1.0 + \delta = 1.0$ on one’s computer.

### 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 8.15: Two Boxes](image)

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

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

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

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

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

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

The probability to find $\phi_1^{(+)}(x)$ is

$$P_{1+} = |\left\langle \phi_1^{(+)} \mid \psi \right\rangle|^2 = \left( \frac{1}{\sqrt{2}} \right)^2 = \frac{1}{2}$$
(b) What is the probability of finding the particle with energy $\frac{\pi^2 \hbar^2}{2ma^2}$?

The probability to find energy $\frac{\pi^2 \hbar^2}{2ma^2}$ is the probability to find eigenvalue $E_1$. There are two eigenfunctions with energy $E_1$, namely, $\phi_1^{(+)}(x)$ and $\phi_1^{(-)}(x)$. We have

$$P_{1+} = |\langle \phi_1^{(+)} | \psi \rangle|^2 = \left( \frac{1}{\sqrt{2}} \right)^2 = \frac{1}{2}$$

$$P_{1-} = |\langle \phi_1^{(-)} | \psi \rangle|^2 = \left( \frac{1}{2} \right)^2 = \frac{1}{4}$$

Therefore, the total probability of $E_1$ is

$$P_{E_1} = \frac{1}{2} + \frac{1}{4} = \frac{3}{4}$$

NOTE: $\phi_1^{(+)}$ and $\phi_1^{(-)}$ are orthogonal so they do not interfere.

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

The probability to be in the left well is

$$P_{\text{left}} = \sum_n |c_n^{(+)}|^2$$

The probability to be in the right well is

$$P_{\text{right}} = \sum_n |c_n^{(-)}|^2$$

where $\psi(x) = \sum_n c_n^{(+)} \phi_n^{(+)} + \sum_n c_n^{(-)} \phi_n^{(-)}$

Thus, for our wave function

$$P_{\text{left}} = \left( \frac{1}{\sqrt{2}} \right)^2 = \frac{1}{2}$$

The probability to be in the right well is

$$P_{\text{right}} = \sum_n |c_n^{(-)}|^2 = \left( \frac{1}{2} \right)^2 + \left( \frac{1}{2} \right)^2 = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$$

so there is a 50-50 chance to find the particle in the left or right well.
(d) What is the state at a later time assuming no measurements are done?

We have
\[ \psi(x,t) = \left( \frac{1}{2} \phi_1^-(x) + \frac{1}{\sqrt{2}} \phi_1^+(x) \right) e^{-iE_1 t/\hbar} + \frac{1}{2} \phi_2^-(x) e^{-iE_2 t/\hbar} \]

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.

We can write the general probability to be ion the left well as
\[ P_{\text{left}}(t) = \sum_n |c_n^+|^2 \]
where
\[ |\psi(t)\rangle = \sum_n c_n^+ e^{-iE_n t/\hbar} |\phi_n^+\rangle + \sum_n c_n^- e^{-iE_n t/\hbar} |\phi_n^-\rangle \]

NOTE: This expansion for \( P_{\text{left}}(t) \) is only valid because \( |\phi_n^+\rangle \) and \( |\phi_n^-\rangle \) are orthogonal, since they do not overlap.

We then have
\[ P_{\text{left}}(t) = \sum_n |c_n^+(t)|^2 = \sum_n |c_n^+e^{-iE_n t/\hbar}|^2 = \sum_n |c_n^+|^2 \]
which is independent of time.

This makes sense physically, since the boxes have infinite depth. There is no way the particle can move from the left to the right, not even by tunneling. 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.

To show that this state is a stationary state we need to show that it is an eigenstate of \( \hat{H} \).
\[ \hat{H} \Phi_n(x) = \hat{H}(c_1 \phi_n^+(x) + c_2 \phi_n^-(x)) = c_1 \hat{H} \phi_n^+(x) + c_2 \hat{H} \phi_n^-(x) = c_1 E_n \phi_n^+(x) + c_2 E_n \phi_n^-(x) = E_n \Phi_n(x) \]

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?

The probability density in $x$ is $|\psi(x)|^2$ as shown below.

\[ \langle x \rangle = 0 \] by inspection. It is time independent (a stationary state).

(h) Show that the momentum space wave function is

\[ \tilde{\psi}(p) = \sqrt{2} \cos \left( \frac{pL}{2\hbar} \right) \tilde{u}_1(p) \]

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 $u_1(x)$.

We have

\[ \tilde{\psi}(p) = \frac{\tilde{\phi}_1^{(+)}(p) + \tilde{\phi}_1^{(-)}(p)}{\sqrt{2}} \]

But

\[ \phi_n^{(\pm)}(x) = u_n(x \pm L/2) \]

Therefore we can use shift-phase duality to write

\[ \tilde{\phi}_n^{(\pm)}(p) = \tilde{u}_n(p) e^{\pm ipL/2\hbar} \]

and thus

\[ \tilde{\psi}(p) = \sqrt{2} \cos \left( \frac{pL}{2\hbar} \right) \tilde{u}(p) \]

Now $\tilde{u}(p)$ is the Fourier transform of

which looks kind of like a top hat. We get something that looks like:
where the red curve is $\tilde{u}(p)$ with $\Delta p \sim \hbar/a$ and the blue curve is $\tilde{\psi}(p)$. The spacing between maxima of $\tilde{\psi}(p)$ is $2\pi$. The $x-$axis is $pL/2\hbar = pa/\hbar$.

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

We have $\langle p \rangle = 0$ by inspection since $\tilde{\psi}(p)$ is symmetric around the origin. This does not change since $\psi(x)$ is a stationary state.

(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.

Suppose $V(x) \to 0$ instantaneously. This implies that the particle is now free. Right after the potential is turned off, $\psi(x)$ is the same state, say

Now the two wave packets spread
Eventually they overlap and interfere.

NOTE: this is just the two-slit problem.

8.15.38 A half-infinite/half-leaky box

Consider a one dimensional potential

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

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

\[ u(x) = \begin{cases} 
0 & x < 0 \\
A \frac{\sin (kx + \phi(k))}{\sin (ka)} \sin (kx) & 0 < x < a \\
A \sin (kx + \phi(k)) & x > a 
\end{cases} \]
where
\[ k = \sqrt{\frac{2mE}{\hbar^2}} , \quad \phi(k) = \tan^{-1}\left[ \frac{k \tan(ka)}{k - \gamma_0 \tan(ka)} \right] , \quad \gamma_0 = \frac{2mU_0}{\hbar^2} \]

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

Solutions to the T.I.S.E., \( \hat{H}u = Eu \) are:

Region \( x < 0 \) : \( u(x) = 0 \) since \( V = \infty \)

Region \( x > a \) : a free particle with general solution
\[ u(x) = A \sin(ka + \phi) \]

Region \( 0 < x < a \), boundary condition \( u(0) = 0 \), which implies that
\[ u(x) = B \sin(kx) \]

where
\[ E = \frac{\hbar^2 k^2}{2m} \rightarrow k = \sqrt{\frac{2mE}{\hbar^2}} \]

There are three unknowns, \( A, B, \phi \). We can eliminate two unknowns through the boundary conditions at \( x = a \)

\[ u \text{ continuous} \rightarrow B \sin(ka) = A \sin(ka + \phi) \rightarrow B = A \frac{\sin(ka + \phi)}{\sin(ka)} \]

\( du/dx \) discontinuous at the delta function
\[ \frac{du}{dx}|_{x=a} - \frac{du}{dx}|_{x=a+} = \frac{2mU_0}{\hbar^2}u(a) \]

or
\[ kA \frac{\sin(ka + \phi)}{\sin(ka)} \cos(ka) - kA \cos(ka + \phi) = \gamma_0 A \sin(ka + \phi) \]

where \( \gamma_0 = \frac{2mU_0}{\hbar^2} \). We then have
\[ k \tan(ka + \phi) \tan(ka) = k - \gamma_0 \tan(ka) \]

or
\[ \phi = \tan^{-1}\left( \frac{k \tan(ka)}{k - \gamma_0 \tan(ka)} \right) - ka \]

These are unbound states since the wave function does not go to zero at \( \infty \).
(b) Show that the limits $\gamma_0 \to 0$ and $\gamma_0 \to \infty$ give reasonable solutions.

The limit as $\gamma_0 \to 0$ is

$$\phi = \tan^{-1} \left( \frac{k \tan (ka)}{k} \right) - ka = ka - ka = 0$$

which implies that

$$u(x) = A \sin kx \quad x > 0$$

The limit $\gamma_0 \to \infty$ gives $\phi = -ka$, which implies that

$$u(x) = 0 \text{ inside} \quad u(x) = A \sin (k(x - a)) \text{ outside}$$

The limit $U_0 \to \infty$ is like an infinite wall at $x = a$, which implies that the wave function goes to zero at $x = a$. Because we have insisted that the wave function be continuous, then $u(x) = 0$ inside the well.

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

When $ka = \pi$, we have $\phi(k) = -ka = -\pi$

Because the wave function is zero at $x = a$, it is invisible to the delta function. This is the quasi-bound resonance.

(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.

When $ka = \pi/2$, 

$$\phi(k) = \tan^{-1} \left( \frac{k}{-\gamma_0} \right) - \frac{\pi}{2}$$

or

$$\frac{\sin (ka + \phi)}{\sin (ka)} = \sin \tan^{-1} \left( \frac{k}{-\gamma_0} \right) < 1$$

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The wave function has a discontinuity in its derivative. Note that inside the "well" the wave function is smaller than in part (c). This is because we are off resonance.

(c) In a scattering scenario, we imagine sending in an incident plane wave which is reflected with unit probability, but phase shifted according to the conventions shown in the figure below:

![Figure 8.17: Scattering Scenario](image)

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.

The wave function for $x > a$

$$u(x) = A \sin(kx + \phi) = A \frac{e^{i(kx+\phi)} - e^{-i(kx+\phi)}}{2i} = -A \frac{e^{-i\phi}}{2i} (e^{-ikx} - e^{ikx+2i\phi})$$

Thus, $\delta = 2\phi$ (the so-called scattering phase shift). The $S$-matrix $\to \infty$ here for the quasi-bound state. For this case, $k$ is complex which implies finite lifetime!

8.15.39 Neutrino Oscillations Redux

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

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

for \( p = |\vec{p}| \). Suppose in a basis of two states, \( m^2 \) is given as a \( 2 \times 2 \) 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 \( m^2 \).

We construct the matrix

\[ m^2 = m_0^2 \{\{1, 0\}, \{0, 1\}\} + \frac{\Delta m^2}{2} \{\{-\cos(2\theta), \sin(2\theta)\}, \{\sin(2\theta), \cos(2\theta)\}\} \]

and solve for the eigenstates

\[ \text{Simplify[Eigensystem}[m^2, \text{Assumptions} \to \{\text{dm}^2 > 0\}] \]

\[ \{\{-\Delta m^2 / 2 + m_0^2, \Delta m^2 / 2 + m_0^2\}, \{-\cot(\theta), 1\}, \{\tan(\theta), 1\}\} \]

We find the normalized eigenvalue/eigenvector pairs

\[ \lambda_- = m_0^2 - \frac{\Delta m^2}{2} , \quad |\nu^-> = \begin{pmatrix} -\cos\theta \\ \sin\theta \end{pmatrix} \]

\[ \lambda_+ = m_0^2 + \frac{\Delta m^2}{2} , \quad |\nu^+> = \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix} \]

(b) Calculate the probability for the state

\[ |\psi> = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]

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

The probability to measure

\[ |\psi(0)> = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]

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at time $t$ is $|\langle \psi(0) | \psi(t) \rangle|^2$, where

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle.$$  

If we write

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\cos \theta |\nu-\rangle + \sin \theta |\nu+\rangle$$

then we may write

$$|\psi(t)\rangle = -\cos \theta |\nu-\rangle e^{-iH_-t/\hbar} + \sin \theta |\nu+\rangle e^{-iH_+t/\hbar}$$

where

$$H_{\pm} = pc + \frac{c^3}{2p} \lambda_{\pm} = pc + \frac{c^3}{2p} \left( m_0^2 \pm \frac{\Delta m^2}{2} \right)$$

The, the probability is

$$|\langle \psi(0) | \psi(t) \rangle|^2 = | -\cos \theta \langle \psi(0) | \nu- \rangle e^{-iH_-t/\hbar} + \sin \theta \langle \psi(0) | \nu+ \rangle e^{-iH_+t/\hbar}|^2$$

$$= | \cos^2 \theta e^{-iH_-t/\hbar} + \sin^2 \theta e^{-iH_+t/\hbar}|^2$$

$$= 1 - \sin^2 (2\theta) \sin^2 (H_+ - H_-) t/2\hbar$$

Inserting the eigenvalues and recognizing that neutrinos are ultra-relativistic,

$$\text{vert} \langle \psi(0) | \psi(t) \rangle|^2 = 1 - \sin^2 (2\theta) \sin^2 \left( \frac{1}{4\hbar c} \left( \Delta m^2 c^4 \right) \frac{t}{E} \right)$$

This can be massaged further to use experimentally convenient units:

$$|\langle \psi(0) | \psi(t) \rangle|^2 = 1 - \sin^2 (2\theta) \sin^2 \left( \frac{1}{4\hbar c} \left( \Delta m^2 c^4 \right) \frac{t}{E} \right)$$

$$= 1 - \sin^2 (2\theta) \sin^2 \left( \frac{1.267 (\Delta m^2 c^4)}{E} \frac{t}{km} \right)$$

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

Let us implement the expression to try to recreate the baseline and periodicity (in units of $\text{km}/\text{MeV}$) in the data:

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Figure 3 in the paper shows a peak-to-peak wavelength of a bit over 30 km/MeV, which is reproduced nicely here with the value of $\Delta m^2 = 8 \times 10^{-5}$ eV$^2$ quoted in the paper. This is not surprising, as their quoted error is only $\pm 0.5 \times 10^{-5}$ eV$^2$.

The amplitude and center of oscillation are more problematic, as this is entirely dependent on $\theta$. The authors quote a range of $0.33 < \tan^2 \theta < 0.5$, which corresponds to $0.75 < \sin^2 \theta < 0.9$; however, this is after including data from solar neutrinos, which puts strong constraints on $\theta$ as shown in Figure 4(a). Looking at the 95% confidence range for just KamiLAND, $0.1 < \tan^2 \theta < 5$, or $0.33 < \sin^2 \theta < 0.56$ passing through $\sin^2 = 1$. Examining Figure 3, the peak and trough are at roughly 1.0 and 0.2 respectively, and this is reproduced above with the quoted value of $\sin^2 \theta 0.8$ ($\tan^2 \theta = 0.4$).

### 8.15.40 Is it in the ground state?

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

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

A particle is placed in the left-hand half of the well so that its wavefunction is $\psi = \text{constant}$ for $x < a/2$. If the energy of the particle is now measured, what is the probability of finding it in the ground state?
The wavefunction is
\[ \psi(x) = \begin{cases} \sqrt{2}a_0 & 0 < x < a/2 \\ 0 & \text{otherwise} \end{cases} \]

The probability for finding it in the ground state is given by
\[ P = |\langle n=1 | \psi(x) \rangle|^2 = |\sqrt{2}a_0 \int_{a/2}^{a} \sin \left( \frac{\pi x}{a} \right) dx|^2 \]

Thus,
\[ P = \left| \frac{2a}{a \pi} \int_{0}^{\pi/2} \sin q dq \right|^2 = \frac{4}{\pi^2} = 0.405 \]

8.15.41 Some Thoughts on T-Violation

Any Hamiltonian can be recast to the form
\[ H = U \begin{pmatrix} E_1 & 0 & \ldots & 0 \\ 0 & E_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & E_n \end{pmatrix} U^+ \]

where \( U \) is a general \( n \times n \) unitary matrix.

(a) Show that the time evolution operator is given by
\[ e^{-iHt/\hbar} = U \left( e^{-iE_1t/\hbar} \begin{pmatrix} 0 & 0 & \ldots & 0 \\ 0 & e^{-iE_2t/\hbar} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & e^{-iE_nt/\hbar} \end{pmatrix} \right) U^+ \]

The time evolution operator is
\[ e^{-iHt/\hbar} = \sum_k \frac{(-it/\hbar)^k}{k!} H^k = \sum_k \frac{(-it/\hbar)^k}{k!} (UEU^+)^k \]

where \( E \) is the diagonal matrix of Hamiltonian eigenvalues \( E_n \) given above.

Expanding a bit further,
\[ e^{-iHt/\hbar} = \sum_k \frac{(-it/\hbar)^k}{k!} (UEU^+)(UEU^+)...(UEU^+)(UEU^+)_k \]

We see that apart from the ends, every \( U^+ \) has a \( U \) to the right of it. Now a matrix is unitary if \( U^+ = U^{-1} \) and \( (U^+)^+ = U \), so the expression simplifies to
\[ e^{-iHt/\hbar} = U \left( \sum_k \frac{(-it/\hbar)^k}{k!} E^k \right) U^+ = U e^{-iEt/\hbar} U^+ \]
or

\[ e^{-iHt/\hbar} = U \begin{pmatrix} e^{-iE_1t/\hbar} & 0 & \cdots & 0 \\ 0 & e^{-iE_2t/\hbar} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{-iE_nt/\hbar} \end{pmatrix} U^+ \]

by the properties of matrix multiplication.

(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 apparent T-violation due to complex phases. NOTE: This is the same problem as the neutrino oscillation (problem 8.39) if you set \( E_i = \sqrt{p^2 c^2 + m^2 c^4} \approx pc + \frac{m^2 c^4}{2p} \) and set all phases to zero.

The probabilities are

\[ P(1 \to 2) = |\langle 2 | e^{-iHt/\hbar} | 1 \rangle|^2 = |\langle 2 | U e^{-iEt/\hbar} U^+ | 1 \rangle|^2 \]

\[ P(2 \to 1) = |\langle 1 | U e^{-iEt/\hbar} U^+ | 2 \rangle|^2 \]

We will demonstrate that there is no \( T \)-violation by showing \( P(1 \to 2) - P(2 \to 1) = 0 \). let us have Mathematica do the work:

```mathematica
U2m = E^\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};
E2m = \begin{pmatrix} E1 & 0 \\ 0 & E2 \end{pmatrix};
amp212 = (0 1).U2m.MatrixExp[-I.E2m.t/\hbar].Transpose[Conjugate[U2m]].\{1,0\};
p12 = ComplexExpand[Conjugate[amp212] * amp212];
amp221 = (1 0).U2m.MatrixExp[-I.E2m.t/\hbar].Transpose[Conjugate[U2m]].\{0,1\};
p211 = ComplexExpand[Conjugate[amp221] * amp221];
TrigExpand[p12 - p211][[1,1]]
```

0
(c) For a three-state problem, however, the time-reversal invariance can be broken. Calculate the difference $P(1 \rightarrow 2) - P(2 \rightarrow 1)$ 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.

Let us proceed in similar fashion as in the two-state problem above:
Indeed, when $\delta \neq 0$, the two probabilities are different.

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

Again, as above, substituting $U \rightarrow U^*$:

\[
\begin{align*}
\text{amp3c12} & = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} . \text{Conjugate}[U3m] . \text{MatrixExp}[-I H3m \cdot t / \hbar] . \text{Transpose}[U3m] . \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \\
p3c12 & = \text{ComplexExpand}[\text{Conjugate}[\text{amp3c12}] \ast \text{amp3c12}] \\
\text{amp3c21} & = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} . \text{Conjugate}[U3m] . \text{MatrixExp}[-I H3m \cdot t / \hbar] . \text{Transpose}[U3m] . \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\
p3c21 & = \text{ComplexExpand}[\text{Conjugate}[\text{amp3c21}] \ast \text{amp3c21}] \\
P(1 \rightarrow 2) & = P(\bar{1} \rightarrow \bar{2}) \\
\text{Simplify}[\text{TrigExpand}[p312 - p3c12]][[1, 1]] \\
\end{align*}
\]

\[
\begin{align*}
& -4 \cos(013)^2 \sin \left( \frac{E1 - E2}{2 \hbar} t \right) \sin \left( \frac{E1 - E3}{2 \hbar} t \right) \\
& \sin \left( \frac{E2 - E3}{2 \hbar} t \right) \sin(6) \sin(2012) \sin(013) \sin(2023) \\
\end{align*}
\]

\[
P(1 \rightarrow 2) - P(\bar{1} \rightarrow \bar{2}) : \\
\text{TrigExpand}[p312 - p3c21][[1, 1]]
\]

\[
0
\]

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 \( \kappa \) as

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

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

Using the form of the wavefunction given in the problem,

\[
\begin{align*}
\psi(-\epsilon) &= A + B \\
\psi(+\epsilon) &= e^{ika}(Ae^{-ika} + Be^{ika}) \\
\psi'(-\epsilon) &= i\kappa(A + B) \\
\psi'(+\epsilon) &= i\kappa e^{ika}(Ae^{-ika} - Be^{ika})
\end{align*}
\]

which we now solve:

```math
msol = Solve[
\{
A + B == e^{ika} (A e^{-ika} + B e^{ika}), \kappa e^{ika} (A e^{-ika} - B e^{ika}) - \kappa (A - B) == \frac{2 m \lambda}{\hbar^2} (A + B) \\
\}, \{B, \kappa\}]
```

Inserting the solution for \( k \) into the phase \( e^{ika} \):

```math
fool = FullSimplify[E^{ika} /. msol, Assumptions -> \{\hbar > 0, m > 0, \lambda > 0, \kappa > 0, a > 0\}]
```

Making the suggested substitution \( d = \hbar^2/m\lambda \):
We can read off the expressions for the two roots:

\[ e^{ika} = \cos ka + \frac{1}{kd} \sin ka \pm \frac{1}{2d} \left[ \sqrt{\cos^2 ka + \frac{1}{(kd)^2} \sin^2 ka - 1} + \frac{1}{kd} \sin 2ka \right] \]

Recognizing that \( \sin 2ka = 2 \sin ka \cos ka \), we may factor the radicand and pull out a \( \sqrt{-1} \) to give:

\[ e^{ika} = \cos ka + \frac{1}{kd} \sin ka \pm i \sqrt{1 - \left( \cos ka + \frac{1}{kd} \sin ka \right)^2} \]

as desired.

(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.

In the limit \( d \to \infty \), which is nothing but a free particle without a potential, we have

\[ e^{ika} = \cos ka + \frac{1}{kd} \sin ka \pm i \frac{2\pi n}{a} \]

and so

\[ \kappa = \pm \left( k + \frac{2\pi n}{a} \right) \]

Equivalently, \( k \) is the momentum modulo \( 2\pi na \). Therefore, \( \kappa \) and hence the energy grow continuously as a function of \( k \). This can be seen numerically with a \( d \) that is large enough:
kplot1 = Plot[-1/a*Log[phase[[1]]]] /. {a \rightarrow 1, \[Phi] \rightarrow 100} /. \[Pi] \rightarrow \pi \[Times] x,
{x, 0, 4}, PlotRange -> (-\[Pi], \[Pi]), AxesLabel -> \{"\[Kappa]a/\pi", "ka"\}];

kplot2 = Plot[-1/a*Log[phase[[2]]]] /. {a \rightarrow 1, \[Phi] \rightarrow 100} /. \[Pi] \rightarrow \pi \[Times] x,
{x, 0, 4}, PlotRange -> (-\[Pi], \[Pi]), AxesLabel -> \{"\[Kappa]a/\pi", "ka"\}];
As we can see, no band gaps – every $\kappa$ has a real $k$.

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

Looking at the equation

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

if the argument of the square root is negative, the LHS becomes pure real and cannot satisfy the equation for real $k$. Therefore, there is no solution when

$$| \cos ka + \frac{1}{kd} \sin ka | > 1$$

When $d$ is finite but large, the combination exceeds 1 for $\kappa a = n\pi + \epsilon (\epsilon > 0)$. This can be seen by expanding it in terms of $\epsilon$,

$$\cos (n\pi + \epsilon) = (-1)^n \left( 1 - \frac{\epsilon^2}{2} + O(\epsilon^4) \right)$$

$$\sin (n\pi + \epsilon) = (-1)^n \left( \epsilon + O(\epsilon^3) \right)$$

or

$$\cos ka + \frac{1}{kd} \sin ka = (-1)^n \left( 1 + \frac{1}{kd} \epsilon - \frac{\epsilon^2}{2} + O(\epsilon^3) \right)$$

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The magnitude exceeds 1 for $0 < \epsilon < 2/n\kappa d \approx 2a/n\pi d$. The gap must exist just above $\kappa = n\pi/a$ for any $n$, while the gap becomes smaller for large $n$. So there exists a band gap at $\kappa = \pm\pi/a$.

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

Let us plot for the given cases as we did in (b), first the weak $d = 3a$:

```
kplotcw1 = Plot[-I/a*Log[phase[[1]]]] /. {a -> 1, d -> 3} /. \[Kappa] -> \[Kappa]*\[Pi],
{x, 0, 4}, PlotRange -> {-Pi, Pi}, AxesLabel -> {"\(\frac{\[Kappa]\ a}{\[Pi]}\)", "ka"} ;
```

\[\text{Diagram}1\]

```
kplotcw2 = Plot[-I/a*Log[phase[[2]]]] /. {a -> 1, d -> 3} /. \[Kappa] -> \[Kappa]*\[Pi],
{x, 0, 4}, PlotRange -> {-Pi, Pi}, AxesLabel -> {"\(\frac{\[Kappa]\ a}{\[Pi]}\)", "ka"} ;
```

\[\text{Diagram2}\]
We see a big gap at $\kappa = 0$, a smaller one at $\kappa = \pi/a$, a yet smaller one at $\kappa = 2\pi/a$, and a gap you can barely see at $\kappa = 3\pi/a$. This is exactly what we predicted in part (c).

Now let us do the strong case $d = a/3$:

```math
kplotcs1 = Plot[-I/a*Log[phase[[1]]] /. {a -> 1, d -> 1/3} /. \kappa \to \pi*x,
{x, 0, 4}, PlotRange -> {-Pi, Pi}, AxesLabel -> {"$\frac{\kappa a}{\pi}$", "ka"}];
```
\begin{verbatim}
In[22]:={kplotcs2 = Plot[-I/a*Log[phase[[2]]]] /. {a → 1, d → 1/3} /. \[Kappa] → \[Kappa] * a,
{x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"\[Kappa]/\[Pi]", "\[Kappa]"}];

Show[kplotcs1, kplotcs2];
\end{verbatim}
Obviously, there is significant distortion from the free case in part (b), with gaps at \( \kappa = n\pi/a \) much bigger than in the weak case above.

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

It is the parity that changes the overall sign of \( k \). This can be seen from the explicit form of the wave function,

\[
\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{for } -a < x < 0
\]

\[
\psi(x) = e^{ika}(Ae^{i\kappa(x-a)} + Be^{-i\kappa(x-a)}) \quad \text{for } 0 < x < a
\]

The parity transformation gives

\[
\psi(x) = e^{ika}(Ae^{i\kappa(-x-a)} + Be^{-i\kappa(-x-a)})
\]

\[
= Be^{i(k+\kappa)a}e^{ikx} + Ae^{i(k-\kappa)a}e^{-ikx}
\]

\[
= A'e^{ikx} + B'e^{-ikx}
\]

and

\[
\psi(x) = Ae^{ikx} + Be^{-ikx}
\]

\[
= e^{-ika}(Be^{i(k+\kappa)a}e^{ik(x-a)} + Ae^{i(k-\kappa)a}e^{-i\kappa(x-a)})
\]

\[
= e^{-ika}(A'e^{ik(x-a)} + B'e^{-i\kappa(x-a)})
\]

respectively. The two wave functions are related by the changes

\[
A \rightarrow A' = Be^{i(k+\kappa)a}
\]

\[
B \rightarrow B' = Ae^{i(k-\kappa)a}
\]

\[
e^{ika} \rightarrow e^{-ika}
\]

This is called \( Z_2 \) symmetry in \( k \).

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.
We start with the definition,

$$e^{O_a} = I + O_a + \frac{1}{2!} O_a^2 + \frac{1}{3!} O_a^3 + \ldots$$

and insert the spectral decomposition

$$O_a = \sum_i \lambda_i P_i$$

This leads to

$$e^{O_a} = I + \sum_i \lambda_i P_i + \frac{1}{2!} \sum_i \lambda_i^2 P_i + \frac{1}{3!} \sum_i \lambda_i^3 P_i + \ldots$$

$$= \sum_i P_i + \sum_i \lambda_i P_i + \frac{1}{2!} \sum_i \lambda_i^2 P_i + \frac{1}{3!} \sum_i \lambda_i^3 P_i + \ldots$$

$$= \sum_i \left( \sum_{n=0}^{\infty} \frac{\lambda_i^n}{n!} \right) P_i$$

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

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

In order to have $\Delta E_A = 0$, it must be the case that $P_i |\Psi_a\rangle = |\Psi_a\rangle$ for some eigenspace projector. Then

$$E_a |\Psi_a\rangle = e^{\lambda_i} |\Psi_a\rangle$$

$$E_a^2 |\Psi_a\rangle = e^{2\lambda_i} |\Psi_a\rangle$$

$$\Delta E_a = 0$$

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 $|\Psi_A(0)\rangle$.

By definition,

$$\Delta O_x = \sqrt{\langle O_x^2 \rangle - \langle O_x \rangle^2}$$
so we start by computing

\[
\langle O_x \rangle = (1\ 0) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (1\ 0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0
\]

Next

\[
O_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

so obviously \( \langle O_x^2 \rangle = 1 \). The finally \( \Delta O_x = 1 \) for 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 \( t \).

We have

\[
\frac{d}{dt} |\Psi_a(t)\rangle = -\frac{i}{\hbar} H |\Psi_a(t)\rangle
\]

\[
|\Psi_a(t)\rangle = e^{-iHt/\hbar} |\Psi_a(0)\rangle
\]

We begin by diagonalizing the Hamiltonian (divided by \( \hbar \)):

\[
\frac{1}{\hbar} H = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}
\]

\[
\lambda^2 - 1 = 0 \rightarrow \lambda = \pm 1
\]

\[
\lambda = +1 \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} \quad \lambda = -1 \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}
\]

\[
\frac{1}{\hbar} H = \frac{1}{2} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix}
\]

Thus,

\[
e^{-iHt/\hbar} = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \left( \frac{1}{\hbar} H \right)^n
\]

\[
= \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \frac{1}{2} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix}
\]

\[
= \frac{1}{2} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \begin{pmatrix} e^{-it} & 0 \\ 0 & e^{it} \end{pmatrix} \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix}
\]

\[
= \frac{1}{2} \begin{pmatrix} e^{-it} + e^{it} & ie^{-it} - ie^{it} \\ -ie^{-it} + ie^{it} & e^{-it} + e^{it} \end{pmatrix}
\]

\[
= \begin{pmatrix} \cos (t) & \sin (t) \\ -\sin (t) & \cos (t) \end{pmatrix}
\]
so

$$| \Psi_a(t) \rangle = \begin{pmatrix} \cos(t) \\ -\sin(t) \end{pmatrix}$$

and at time $t$,

$$\langle O_x \rangle \rightarrow (\cos(t) - \sin(t)) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos(t) \\ -\sin(t) \end{pmatrix} = (\cos(t) - \sin(t)) \begin{pmatrix} -\sin(t) \\ \cos(t) \end{pmatrix} = -2\sin(t)\cos(t) = -\sin(2t)$$

$$\langle O_x^2 \rangle = 1$$

$$\Delta O_x = \sqrt{1 - \sin^2(2t)} = |\cos(2t)|$$

(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 $\Delta O_Z$ as a function of $t$ assuming evolution according to the Schrodinger equation with the Hamiltonian above.

Noting $O_Z^2$ is again the identity, we compute at time $t$

$$\langle O_z \rangle \rightarrow (\cos(t) - \sin(t)) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos(t) \\ -\sin(t) \end{pmatrix} = (\cos(t) - \sin(t)) \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix} = \cos^2(t) - \sin^2(t) = \cos(2t)$$

$$\langle O_z^2 \rangle = 1$$

$$\Delta O_z = \sqrt{1 - \sin^2(2t)} = |\cos(2t)|$$

(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?
We have
\[
[O_x, O_z] = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
= \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\
= \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix}
\]
so at time \( t \)
\[
\langle [O_x, O_z] \rangle = (\cos(t) - \sin(t)) \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} (\cos(t)) \\
= (\cos(t) - \sin(t)) \begin{pmatrix} 2 \sin(t) \\ 2 \cos(t) \end{pmatrix} \\
= 0
\]
Hence with
\[
\Delta O_x \Delta O_z = |\sin(2t)||\cos(2t)|
\]
we see that the relation is always satisfied. The product of the uncertainties actually reaches zero whenever either \( \Delta O_x \) or \( \Delta O_z \) vanishes, i.e.,
\[
t = \frac{n\pi}{4}, \quad n = 0, 1, 2, ....
\]
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

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

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

We have

$$\psi(\theta, \phi) = \sqrt{\frac{15}{8\pi}} \cos \theta \sin \theta \cos \phi = \sqrt{\frac{15}{8\pi}} \cos \theta \sin \theta \left( \frac{e^{i\phi} + e^{-i\phi}}{2} \right)$$

Now

$$Y_{2,\pm 1}(\theta, \phi) = \pm \sqrt{\frac{15}{8\pi}} \cos \theta \sin \theta e^{\pm i\phi}$$

so that

$$\psi(\theta, \phi) = \frac{1}{2} (-Y_{2,1}(\theta, \phi) + Y_{2,-1}(\theta, \phi))$$

or

$$|\psi\rangle = \frac{1}{2} (-|2, 1\rangle + |2, -1\rangle)$$ using then notation \(|L, L_z\rangle\)

The state is not normalized, that is,

$$\langle \psi | \psi \rangle = \frac{1}{4} (1 + 1) = \frac{1}{2}$$

so after proper normalization we have

$$|\psi\rangle = \frac{1}{\sqrt{2}} (-|2, 1\rangle + |2, -1\rangle)$$
It is clear from the state vector that

\[ L_z = \pm 1 \] each with probability \( = 1/2 \)

We then have

\[ \langle L_z \rangle = \hbar P(L_z = +1) - \hbar P(L_z = -1) = 0 \]

For completeness, let us also do this calculation in the position representation. We have

\[ \langle L_z \rangle = \int \int \psi^* \hat{L}_z \psi \sin \theta d\theta d\varphi \]

\[ = \int \int \frac{1}{\sqrt{2}} (Y_{2,-1}^* - Y_{2,1}^*) \hat{L}_z \frac{1}{\sqrt{2}} (Y_{2,-1} - Y_{2,1}) d\Omega \]

\[ = \frac{\hbar}{2} \int \int (Y_{2,-1}^* - Y_{2,1}^*) (-Y_{2,-1} - Y_{2,1}) d\Omega \]

\[ = \frac{\hbar}{2} \left[ - \int \int Y_{2,-1}^* Y_{2,-1}^* d\Omega + \int \int Y_{2,1}^* Y_{2,1}^* d\Omega \right] = \frac{\hbar}{2} [-1 + 1] = 0 \]

where we have used the orthonormality of the spherical harmonics.

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

We have

\[ \hat{L}_x = \frac{\hat{L}_+ + \hat{L}_-}{2} \]

so that

\[ \langle L_x \rangle = \frac{1}{\sqrt{2}} (\langle 2, 1 \rangle + \langle 2, -1 \rangle) \frac{\hat{L}_+ + \hat{L}_-}{2} \frac{1}{\sqrt{2}} (\langle 2, 1 \rangle + \langle 2, -1 \rangle) = \frac{1}{4}(0) = 0 \]

since all the matrix elements are identically zero.

### 9.7.2 Operator identities

Show that

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

We have

\[ [\vec{a}, \vec{b}] = [\vec{a}, \vec{L}] = [\vec{b}, \vec{L}] = 0 \]

Using Einstein summation convention we have

\[ [\vec{a} \cdot \vec{L}, \vec{b} \cdot \vec{L}] = (\vec{a} \cdot \vec{L})(\vec{b} \cdot \vec{L}) - (\vec{b} \cdot \vec{L})(\vec{a} \cdot \vec{L}) \]

\[ = (a_i L_i)(b_j L_j) - (b_j L_j)(a_i L_i) \]

\[ = a_i b_j [L_i, L_j] = a_i b_j i\hbar \varepsilon_{ijk} L_k \]

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

Again using Einstein summation convention we have
\[
\left[ \vec{L}^2, \vec{V} \right] = \left[ \hat{L}_m \hat{L}_m, \hat{V}_n \hat{V}_n \right] = \hat{L}_m \hat{L}_m \hat{V}_n - \hat{V}_n \hat{L}_m \hat{L}_m \\
= \hat{V}_n \hat{L}_m \left( \hat{L}_m \hat{V}_n + \hat{V}_n \hat{L}_m \right) - \left( \hat{L}_m \hat{V}_n - \hat{L}_m \hat{V}_n \right) \hat{L}_m \\
= \hat{V}_n \hat{L}_m \hat{L}_m \hat{V}_n + \left( \hat{L}_m \hat{V}_n \right) \hat{L}_m
\]

Now for any vector operator we have
\[
\left[ \hat{L}_m, \hat{V}_n \right] = i\hbar \varepsilon_{mnp} \hat{V}_p
\]

so that
\[
\left[ \vec{L}^2, \vec{V} \right] = \hat{V}_n \hat{L}_m \left[ \hat{L}_m, \hat{V}_n \right] + \left[ \hat{L}_m, \hat{V}_n \hat{L}_m \right] \\
= i\hbar \varepsilon_{mnp} \left[ \hat{L}_m \hat{V}_p + \hat{V}_p \hat{L}_m \right] = i\hbar \left( \vec{V} \times \vec{L} - \vec{L} \times \vec{V} \right)
\]

Now consider
\[
\left( \vec{L} \times \vec{V} \right)_1 = L_2 V_3 - L_3 V_2 = (V_3 L_2 + iV_1) - (V_2 L_3 - iV_1)
\]

where we have used
\[
\left[ \hat{L}_m, \hat{V}_n \right] = i\hbar \varepsilon_{mnp} \hat{V}_p
\]

Thus,
\[
\left( \vec{L} \times \vec{V} \right)_1 = - \left( \vec{V} \times \vec{L} \right)_1 + 2iV_1
\]
or
\[
\vec{L} \times \vec{V} = \vec{V} \times \vec{L} + 2i\hbar \vec{V} \text{ for operators}
\]

Therefore,
\[
\left[ \vec{L}^2, \vec{V} \right] = i\hbar \left( \vec{V} \times \vec{L} - \vec{L} \times \vec{V} \right) = 2i\hbar \left( \vec{V} \times \vec{L} - i\hbar \vec{V} \right)
\]

### 9.7.3 More operator identities

Prove the identities

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

Using Einstein summation convention we have
\[
\left( \hat{\sigma} \cdot \hat{A} \right) \left( \hat{\sigma} \cdot \hat{B} \right) = A_i B_j \hat{\sigma}_i \hat{\sigma}_j = A_i B_j \left( \delta_{ij} + i\varepsilon_{ijk} \hat{\sigma}_k \right) \\
= A_i B_j \delta_{ij} + i\varepsilon_{ijk} A_i B_j \hat{\sigma}_k = \hat{A} \cdot \hat{B} + i\hat{\sigma} \cdot \left( \hat{A} \times \hat{B} \right)
\]

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

Again using Einstein summation convention we have
\[
e^{i\phi \vec{S} \cdot \hat{n} / \hbar} e^{-i\phi \vec{S} \cdot \hat{n} / \hbar} = e^{i\phi \vec{\sigma} \cdot \hat{n} / 2\hbar} e^{-i\phi \vec{\sigma} \cdot \hat{n} / 2\hbar}
\]
and
\[
e^{i\phi \vec{\sigma} \cdot \hat{n} / 2\hbar} = \cos \frac{\phi}{2} \hat{I} + i \hat{\sigma} \cdot \hat{n} \sin \frac{\phi}{2}
\]
Therefore,
\[
e^{i\phi \vec{S} \cdot \hat{n} / \hbar} e^{-i\phi \vec{S} \cdot \hat{n} / \hbar} = \left( \cos \frac{\phi}{2} \hat{I} + i \hat{\sigma} \cdot \hat{n} \sin \frac{\phi}{2} \right) \vec{\sigma} \left( \cos \frac{\phi}{2} \hat{I} - i \hat{\sigma} \cdot \hat{n} \sin \frac{\phi}{2} \right)
\]
\[
= \cos^2 \frac{\phi}{2} \vec{\sigma} + i \sin \frac{\phi}{2} \cos \frac{\phi}{2} [\vec{\sigma} \cdot \hat{n}, \vec{\sigma}] + \sin^2 \frac{\phi}{2} (\vec{\sigma} \cdot \hat{n}) \vec{\sigma} (\vec{\sigma} \cdot \hat{n})
\]
Now
\[
[\vec{\sigma} \cdot \hat{n}, \vec{\sigma}] = n_i \hat{e}_j [\sigma_i, \sigma_j] = 2i n_i \hat{e}_j \epsilon_{ijk} \sigma_k = 2i \epsilon_{ki} \sigma_j n_i \hat{e}_j = 2i (\vec{\sigma} \times \hat{n})
\]
and
\[
(\vec{\sigma} \cdot \hat{n}) \vec{\sigma} (\vec{\sigma} \cdot \hat{n}) = n_i n_k \hat{e}_j \delta_i \delta_j \delta_k = n_i n_k \hat{e}_j \delta_i \delta_j (\delta_{jk} + i \epsilon_{jkm} \delta_m)
\]
\[
= n_i n_k \hat{e}_j \delta_i \delta_j + i \epsilon_{jkm} n_i n_j \hat{e}_k \delta_i \delta_m
\]
\[
= n_i n_j \hat{e}_j \delta_i + i \epsilon_{jkm} n_i n_j \hat{e}_k \delta_i \delta_m
\]
\[
= \hat{n} (\vec{\sigma} \cdot \hat{n}) + i \epsilon_{jkm} n_i n_j \hat{e}_k \delta_i \delta_m
\]
\[
= \hat{n} (\vec{\sigma} \cdot \hat{n}) + i \epsilon_{jkm} n_i n_j \hat{e}_k \delta_i \delta_m
\]
\[
= \hat{n} (\vec{\sigma} \cdot \hat{n}) + n_i \hat{e}_i \vec{\sigma} (\vec{\sigma} \cdot \hat{n}) - \vec{\sigma} (\vec{\sigma} \cdot \hat{n}) = 2 \hat{n} (\vec{\sigma} \cdot \hat{n}) - \vec{\sigma}
\]
Now
\[
\hat{n} \times (\hat{n} \times \vec{\sigma}) = (\hat{n} \cdot \vec{\sigma}) \hat{n} - (\vec{\sigma} \cdot \hat{n}) \hat{n} \rightarrow \vec{\sigma} = (\vec{\sigma} \cdot \hat{n}) \hat{n} + \hat{n} \times (\hat{n} \times \vec{\sigma})
\]
so that
\[
(\vec{\sigma} \cdot \hat{n}) \vec{\sigma} (\vec{\sigma} \cdot \hat{n}) = 2 \hat{n} (\vec{\sigma} \cdot \hat{n}) - \vec{\sigma} = (\vec{\sigma} \cdot \hat{n}) \hat{n} - \hat{n} \times (\hat{n} \times \vec{\sigma})
\]
Finally,
\[
e^{i\phi \vec{S} \cdot \hat{n} / \hbar} e^{-i\phi \vec{S} \cdot \hat{n} / \hbar} = \cos^2 \frac{\phi}{2} + i \sin \frac{\phi}{2} \cos \frac{\phi}{2} [\vec{\sigma} \cdot \hat{n}, \vec{\sigma}] + \sin^2 \frac{\phi}{2} (\vec{\sigma} \cdot \hat{n}) \vec{\sigma} (\vec{\sigma} \cdot \hat{n})
\]
\[
= \cos^2 \frac{\phi}{2} (\vec{\sigma} \cdot \hat{n} + \hat{n} \times (\hat{n} \times \vec{\sigma})) - 2 \sin \frac{\phi}{2} \cos \frac{\phi}{2} (\vec{\sigma} \times \hat{n})
\]
\[
+ \sin^2 \frac{\phi}{2} ((\vec{\sigma} \cdot \hat{n}) \hat{n} - \hat{n} \times (\hat{n} \times \vec{\sigma}))
\]
\[
= (\vec{\sigma} \cdot \hat{n}) \hat{n} + (\hat{n} \times (\hat{n} \times \vec{\sigma})) \cos \phi + \sin \phi (\hat{n} \times \vec{\sigma})
\]
}\[
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\]
9.7.4 On a circle

Consider a particle of mass \( \mu \) 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.

We have the potential \( V = 0 \) and the kinetic energy

\[
T = \frac{1}{2} \mu v^2 = \frac{1}{2} \mu a^2 \dot{\phi}^2 \quad , \quad v = a \dot{\phi}
\]

In addition,

\[
L_z = \mu a v = \mu a^2 \dot{\phi}
\]

so that

\[
H = T + V = \frac{L^2}{2\mu a^2}
\]

Now we have

\[
H \left| \psi \right\rangle = \frac{L_z^2}{2\mu a^2} \left| \psi \right\rangle = E \left| \psi \right\rangle
\]

or

\[
\langle \phi | H | \psi \rangle = \langle \phi | \frac{L_z^2}{2\mu a^2} | \psi \rangle = \langle \phi | E | \psi \rangle
\]

\[
\frac{1}{2\mu a^2} \left( \frac{\hbar}{\tau} \frac{\partial}{\partial \phi} \right)^2 \langle \phi | \psi \rangle = \frac{h}{2\mu} \frac{\partial^2 \psi(\phi)}{\partial \phi^2} = E \psi(\phi)
\]

so that we have the solution

\[
\psi(\phi) = A e^{im\phi} \quad , \quad E = \frac{\hbar^2 m^2}{2\mu a^2}
\]

Now, imposing single-valuedness, we have

\[
\psi(\phi) = A e^{im\phi} = \psi(\phi + 2\pi) = A e^{im\phi} e^{i2\pi m}
\]

\[
e^{i2\pi m} = 1 \rightarrow m = \text{integer}
\]

Since \( m \) and \(-m\) give the same energy, each level is 2-fold degenerate, corresponding to rotation CW and CCW.

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 \( \omega_0 \) is a constant. If

\[
\langle \theta, \phi | \psi(0) \rangle = \sqrt{\frac{3}{4\pi}} \sin \theta \sin \phi
\]
what is $\langle \theta, \phi \mid \psi(t) \rangle$? What is $\hat{L}_x$ at time $t$?

Preliminary work:

$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi} = -\sqrt{\frac{3}{8\pi}} \frac{x+iy}{r}$$
$$Y_{1,-1} = \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi} = \sqrt{\frac{3}{8\pi}} \frac{x-iy}{r}$$

Now

$$\langle \theta, \phi \mid \psi(0) \rangle = \sqrt{\frac{3}{4\pi}} \sin \theta \sin (\phi) = \sqrt{\frac{3}{4\pi}} \sin \theta e^{i\phi}$$

or

$$|\psi(0)\rangle = \frac{i}{\sqrt{2}} |1, 1\rangle + \frac{i}{\sqrt{2}} |1, -1\rangle$$

Now,

$$\hat{H} = \frac{\hat{L}_x^2}{2I} + \omega_0 \hat{L}_z$$

and

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = \frac{i}{\sqrt{2}} e^{-iE_{1,1}t/\hbar} |1, 1\rangle + \frac{i}{\sqrt{2}} e^{-iE_{1,-1}t/\hbar} |1, -1\rangle$$

where

$$\hat{H} |L, M\rangle = \frac{\hat{L}_x^2}{2I} |L, M\rangle + \omega_0 \hat{L}_z |L, M\rangle = \left( \frac{\hbar^2}{2I} L(L+1) + M\omega_0 \right) |L, M\rangle = E_{L,M} |L, M\rangle$$

Therefore,

$$|\psi(t)\rangle = \frac{i}{\sqrt{2}} e^{-iE_{1,1}t/\hbar} |1, 1\rangle + \frac{i}{\sqrt{2}} e^{-iE_{1,-1}t/\hbar} |1, -1\rangle = \frac{i}{\sqrt{2}} e^{-i\frac{\hbar}{2}t} \left( e^{-i\omega_0 t} |1, 1\rangle + e^{i\omega_0 t} |1, -1\rangle \right)$$

so that

$$\langle \theta, \phi \mid \psi(t) \rangle = \frac{i}{\sqrt{2}} e^{-i\frac{\hbar}{2}t} \left( e^{-i\omega_0 t} Y_{1,1} + e^{i\omega_0 t} Y_{1,-1} \right)$$

$$= \frac{i}{\sqrt{2}} e^{-i\frac{\hbar}{2}t} \sqrt{\frac{3}{8\pi}} \sin \theta \left( e^{-i\omega_0 t} e^{i\phi} + e^{i\omega_0 t} e^{-i\phi} \right)$$

$$= e^{-i\frac{\hbar}{2}t} \sqrt{\frac{3}{4\pi}} \sin \theta (\sin (\phi - \omega_0 t))$$

Finally,

$$\left\langle \hat{L}_x \right\rangle_t = \langle \psi(t) \mid \hat{L}_x \mid \psi(t) \rangle = \frac{1}{2} \langle \psi(t) \mid (\hat{L}_+ + \hat{L}_-) \mid \psi(t) \rangle = 0$$

since states making up $|\psi(t)\rangle$ have $\Delta M = 0, \pm 2$ only.
9.7.6 A Wave Function

A particle is described by the wave function

$$\psi(\rho, \phi) = Ae^{-\rho^2/2\Delta} \cos^2 \phi$$

Determine $P(L_z = 0)$, $P(L_z = 2\hbar)$ and $P(L_z = -2\hbar)$.

We have

$$\psi(\rho, \phi) = Ae^{-\rho^2/2\Delta} \cos^2 \phi = Ae^{-\rho^2/2\Delta} \left(\frac{e^{i\phi} + e^{-i\phi}}{2}\right)^2$$

This corresponds to

$$|\psi\rangle = \left(\frac{1}{\sqrt{6}}|L_z = 1\rangle + \frac{2}{\sqrt{6}}|L_z = 0\rangle + \frac{1}{\sqrt{6}}|L_z = -1\rangle\right)$$

Therefore, we have

$$P(L_z = 0|\psi) = |\langle L_z = 0 | \psi\rangle|^2 = \frac{2}{3}$$
$$P(L_z = +2|\psi) = |\langle L_z = +2 | \psi\rangle|^2 = \frac{1}{6}$$
$$P(L_z = -2|\psi) = |\langle L_z = -2 | \psi\rangle|^2 = \frac{1}{6}$$

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?

Since $L_z$ is diagonal, we are in the $L_z$ basis and the diagonal elements are the $L_z$ eigenvalues, we have, $L_z = 1, 0$. The corresponding eigenvectors are

$$|L_z = +1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |1\rangle, \quad |L_z = -1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = |-1\rangle, \quad |L_z = 0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = |0\rangle$$

(b) Take the state in which $L_z = 1$. In this state, what are $\langle L_z \rangle$, $\langle L_z^2 \rangle$ and $\Delta L_x = \sqrt{\langle L_z^2 \rangle - \langle L_z \rangle^2}$. 

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We have

\[ \langle L_x \rangle = \langle 1 | L_x | 1 \rangle = (1, 0, 0) \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = 0 \]

\[ \langle L_x^2 \rangle = \langle 1 | L_x^2 | 1 \rangle = (1, 0, 0) \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2} \]

\[ \Delta L_x = \sqrt{\langle L_x^2 \rangle - \langle L_x \rangle^2} = \sqrt{1/2} = 0.707 \]

(c) Find the normalized eigenstates and eigenvalues of \( L_x \) in the \( L_z \) basis.

We use

\[ \det [L_x - \lambda I] = 0 = -\lambda^3 + \lambda \rightarrow \lambda = \pm 1, 0 \]

or we get the same eigenvalues as for \( L_z \) as expected. To find the eigenvectors we solve the equations generated by

\[ L_x |L_x = 1\rangle = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \]

or

\[ \frac{1}{\sqrt{2}} b = a \quad , \quad \frac{1}{\sqrt{2}} a + \frac{1}{\sqrt{2}} c = b \quad , \quad \frac{1}{\sqrt{2}} b = c \]

which give

\[ a = c \text{ and } \sqrt{2}a = b \]

Normalization requires that \( a^2 + b^2 + c^2 = 4a^2 = 1 \) so we finally obtain

\[ a = c = \frac{1}{2} \text{ and } b = \frac{1}{\sqrt{2}} \]

\[ |L_x = 1\rangle = \begin{pmatrix} 1/2 \\ 1/\sqrt{2} \\ 1/2 \end{pmatrix} = \frac{1}{2} |L_z = 1\rangle + \frac{1}{\sqrt{2}} |L_z = 0\rangle + \frac{1}{2} |L_z = -1\rangle \]

Similarly, we get

\[ |L_x = -1\rangle = \begin{pmatrix} 1/2 \\ -1/\sqrt{2} \\ 1/2 \end{pmatrix} = \frac{1}{2} |L_z = 1\rangle - \frac{1}{\sqrt{2}} |L_z = 0\rangle + \frac{1}{2} |L_z = -1\rangle \]

\[ |L_x = 0\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} |L_z = 1\rangle - \frac{1}{\sqrt{2}} |L_z = -1\rangle \]

(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?
We have
\[ P(L_x = 1|L_z = -1) = |\langle L_x = 1 \mid L_z = -1 \rangle|^2 = \frac{1}{4} \]
\[ P(L_x = 0|L_z = -1) = |\langle L_x = 0 \mid L_z = -1 \rangle|^2 = \frac{1}{2} \]
\[ P(L_x = -1|L_z = -1) = |\langle L_x = -1 \mid L_z = -1 \rangle|^2 = \frac{1}{4} \]

(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?

We have
\[ |\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1\end{pmatrix} = \frac{1}{2} |L_z = 1\rangle + \frac{1}{2} |L_z = 0\rangle + \frac{1}{\sqrt{2}} |L_z = -1\rangle \]

Now we have
\[ L_z^2 |L_z = 1\rangle = |L_z = 1\rangle \rightarrow \text{eigenvalue } = +1 \]
\[ L_z^2 |L_z = 0\rangle = 0 \rightarrow \text{eigenvalue } = 0 \]
\[ L_z^2 |L_z = -1\rangle = |L_z = -1\rangle \rightarrow \text{eigenvalue } = +1 \]

and
\[ P(L_z = 1|\psi) = |\langle L_z = 1 \mid \psi \rangle|^2 = \frac{1}{4} \]
\[ P(L_z = 0|\psi) = |\langle L_z = 0 \mid \psi \rangle|^2 = \frac{1}{2} \]
\[ P(L_z = -1|\psi) = |\langle L_z = -1 \mid \psi \rangle|^2 = \frac{1}{2} \]

so written in the $L_z^2$ basis states labeled by $|L_z^2, L_z\rangle$ we have
\[ |\psi\rangle = \frac{1}{2} |1, 1\rangle + \frac{1}{2} |0, 0\rangle + \frac{1}{\sqrt{2}} |1, -1\rangle \]

If we measure $L_z^2 = 1$, the new state is
\[ |\psi_{new}\rangle = \frac{1}{\sqrt{3}} |1, 1\rangle + \frac{\sqrt{2}}{3} |1, -1\rangle \]
so that
\[ L_z^2 |\psi_{new}\rangle = |\psi_{new}\rangle \rightarrow \text{eigenvalue } = +1 \]

and
\[ P(L_z^2 = 1|\psi) = |\langle L_z^2 = 1 \mid L_z = 1 \rangle|^2 + |\langle L_z^2 = 1 \mid L_z = 0 \rangle|^2 + |\langle L_z^2 = 1 \mid L_z = -1 \rangle|^2 = \frac{1}{4} + \frac{1}{2} + \frac{3}{4} = 1 \]
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, $P(L_x = 0)$.

Since the phase factor does not affect absolute values, we have, for

$$|\psi\rangle = \frac{e^{i\delta_1}}{2} |L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}} |L_z = 0\rangle + \frac{e^{i\delta_3}}{2} |L_z = -1\rangle$$

$$P(L_z = 1|\psi) = |\langle L_z = 1 | \psi \rangle|^2 = \frac{1}{4}$$

$$P(L_z = 0|\psi) = |\langle L_z = 0 | \psi \rangle|^2 = \frac{1}{4}$$

$$P(L_z = -1|\psi) = |\langle L_z = -1 | \psi \rangle|^2 = \frac{1}{2}$$

as before.

Phase factors (or really relative phases) matter, however, for some measurements. If I write $|\psi\rangle$ in the $|x\rangle$ basis we get

$$|\psi\rangle = \frac{e^{i\delta_1} - e^{i\delta_3}}{2\sqrt{2}} |L_x = 0\rangle + ............$$

so that

$$\langle L_x = 0 | \psi \rangle = \frac{e^{i\delta_1} - e^{i\delta_3}}{2\sqrt{2}}$$

and hence

$$P(L_x = 0|\psi) = |\langle L_x = 0 | \psi \rangle|^2 = \frac{e^{i\delta_1} - e^{i\delta_3}}{2\sqrt{2}}^2 = \frac{1}{4} (1 - \cos (\delta_1 - \delta_3))$$

so clearly relative phase matters.

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 $j_z$, $|m = \pm 3/2\rangle, |m = \pm 1/2\rangle$ and $|m = -3/2\rangle$.,
We have

\[ \hat{J}^2 |3/2, 3/2\rangle = \hbar^2 (3/2)(3/2 + 1) |3/2, 3/2\rangle = 15\hbar^2/4 |3/2, 3/2\rangle \\
\hat{J}^2 |3/2, 3/2\rangle = 3\hbar/2 |3/2, 3/2\rangle \\
\hat{J}^2 |3/2, 1/2\rangle = \hbar^2 (3/2)(3/2 + 1) |3/2, 1/2\rangle = 15\hbar^2/4 |3/2, 1/2\rangle \\
\hat{J}_z |3/2, 1/2\rangle = \hbar/2 |3/2, 1/2\rangle \\
\hat{J}^2 |3/2, -1/2\rangle = \hbar^2 (3/2)(3/2 + 1) |3/2, -1/2\rangle = 15\hbar^2/4 |3/2, -1/2\rangle \\
\hat{J}_z |3/2, -1/2\rangle = -\hbar/2 |3/2, -1/2\rangle \\
\hat{J}^2 |3/2, -3/2\rangle = \hbar^2 (3/2)(3/2 + 1) |3/2, -3/2\rangle = 15\hbar^2/4 |3/2, -3/2\rangle \\
\hat{J}_z |3/2, -3/2\rangle = -3\hbar/2 |3/2, -3/2\rangle \\

The operators \( \hat{J}_\pm \) must satisfy

\[ \hat{J}_\pm |j, j_z\rangle = \hbar \sqrt{j(j+1) - j_z(j_z \pm 1)} |j, j_z \pm 1\rangle \]

(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.

For the operator

\[ \hat{j}_+ = \hbar \left( \sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |1/2\rangle \langle -3/2| \right) \]

we have

\[ \hat{j}_+ |3/2, 3/2\rangle = \hbar \left( \sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |1/2\rangle \langle -3/2| \right) |3/2, 3/2\rangle \\
= 0 = \hbar \sqrt{3}/2(3/2 + 1) - 3/2(3/2 + 1) |3/2, 3/2\rangle \\
\hat{j}_+ |3/2, 1/2\rangle = \hbar \left( \sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |1/2\rangle \langle -3/2| \right) |3/2, 1/2\rangle \\
= \sqrt{3}\hbar |3/2, 3/2\rangle = \hbar \sqrt{3}/2(3/2 + 1) - 1/2(1/2 + 1) |3/2, 3/2\rangle \\
\hat{j}_+ |3/2, -1/2\rangle = \hbar \left( \sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |1/2\rangle \langle -3/2| \right) |3/2, -1/2\rangle \\
= 2\hbar |3/2, 1/2\rangle = \hbar \sqrt{3}/2(3/2 + 1) + 1/2(1/2 + 1) |3/2, 1/2\rangle \\
\hat{j}_+ |3/2, -3/2\rangle = \hbar \left( \sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |1/2\rangle \langle -3/2| \right) |3/2, -3/2\rangle \\
= \sqrt{3}\hbar |3/2, -1/2\rangle = \hbar \sqrt{3}/2(3/2 + 1) + 3/2(-3/2 + 1) |3/2, -3/2\rangle \\
\]

so that the raising operator in this 4-dimensional space is

\[ \hat{j}_+ = \hbar \left( \sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |1/2\rangle \langle -3/2| \right) \]

(b) What is the lowering operator \( \hat{j}_- \)?
We have

\[ \hat{J}_- = (\hat{J}_+)^+ = \hbar \left( \sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle 1/2| + \sqrt{3} |1/2\rangle \langle -3/2| \right)^+ \]

\[ = \hbar \left( \sqrt{3} |1/2\rangle \langle 3/2| + 2 |1/2\rangle \langle 1/2| + \sqrt{3} |1/2\rangle \langle -1/2| \right) \]

(c) What are the matrix representations of \( \hat{J}_x, \hat{J}_y, \hat{J}_z \) and \( \hat{J}^2 \) in the \( J_z \) basis?

\( \hat{J}_z \) and \( J_z \) are both diagonal

\[ \hat{J}_z = \hbar \left( \begin{array}{cccc} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{array} \right) \]

The other operators are not diagonal,

\[ \hat{J}_+ = \hbar \left( \begin{array}{cccc} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{array} \right), \quad \hat{J}_- = \hbar \left( \begin{array}{cccc} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{array} \right) \]

and

\[ \hat{J}_x = \frac{\hat{J}_+ + \hat{J}_-}{2} = \frac{\hbar}{2} \left( \begin{array}{cccc} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{array} \right) \]

\[ \hat{J}_y = \frac{\hat{J}_+ - \hat{J}_-}{2i} = \frac{\hbar}{2i} \left( \begin{array}{cccc} 0 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 0 & 2 & 0 \\ 0 & -2 & 0 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 0 \end{array} \right) \]

(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 \( \hbar/2 \).

We have

\[ |\psi\rangle = \frac{1}{2\sqrt{2}} \left( \sqrt{3} |3/2\rangle + = |1/2\rangle - |1/2\rangle - \sqrt{3} |3/2\rangle \right) = \frac{1}{2\sqrt{2}} \left( \begin{array}{c} \sqrt{3} \\ 1 \\ -1 \\ -\sqrt{3} \end{array} \right) \]

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in the standard basis. The state is normalized since
\[ \langle \psi | \psi \rangle = \frac{1}{8} \left( \sqrt{3} \ 1 \ -1 \ -\sqrt{3} \right) \left( \begin{array}{c} \sqrt{3} \\ 1 \\ -1 \\ -\sqrt{3} \end{array} \right) = \frac{1}{8} (3 + 1 + 1 + 3) = 1 \]

We also have
\[ \hat{J}_x |\psi\rangle = \frac{1}{2\sqrt{2}} \hbar \left( \begin{array}{cccc} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{array} \right) \left( \begin{array}{c} \sqrt{3} \\ 1 \\ -1 \\ -\sqrt{3} \end{array} \right) = \frac{\hbar}{4\sqrt{2}} \left( \begin{array}{c} \sqrt{3} \\ 1 \\ -1 \\ -\sqrt{3} \end{array} \right) |\psi\rangle = \frac{\hbar}{2} |\psi\rangle \]

so it is an eigenvector of \( \hat{J}_x \) with eigenvalue \( \hbar/2 \).

(e) Find the eigenstate of \( \hat{J}_x \) with eigenvalue \( 3\hbar/2 \).

We have
\[ \hat{J}_x |\psi_{3/2}\rangle = \frac{\hbar}{2} \left( \begin{array}{cccc} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{array} \right) \left( \begin{array}{c} a \\ b \\ c \\ d \end{array} \right) = \frac{\hbar}{2} \left( \begin{array}{c} \sqrt{3}b \\ \sqrt{3a + 2c} \\ 2b + \sqrt{3d} \\ \sqrt{3c} \end{array} \right) |\psi\rangle = \frac{3\hbar}{2} |\psi_{3/2}\rangle = \frac{3\hbar}{2} \left( \begin{array}{c} a \\ b \\ c \\ d \end{array} \right) \]

\( \sqrt{3}b = 3a \)
\( \sqrt{3a + 2c} = 3b \)
\( 2b + \sqrt{3d} = 3c \) \( \Rightarrow b = c = \sqrt{3}a = \sqrt{3}d \) \( \Rightarrow |\psi_{3/2}\rangle = \frac{1}{2\sqrt{2}} \left( \begin{array}{c} 1 \\ \sqrt{3} \\ \sqrt{3} \\ 1 \end{array} \right) \)

(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 \( \mu_N \) 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 \( \hat{J}_y \) as a function of time if
\[ \hat{H} = -\vec{\mu} \cdot \vec{B} = -g_N \mu_N \hbar \hat{J}_x \cdot \vec{B} \hat{y} = -g_N \mu_N \hbar B \hat{J}_y \]
where \( \mu_N = e\hbar/2Mc = \) nuclear magneton? You will need to use the identity we derived earlier
\[ e^{x\hat{A}} e^{-x\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] x + [\hat{A}, [\hat{A}, \hat{B}]] \frac{x^2}{2} + [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] \frac{x^3}{6} + \ldots \]
We suppose at $t = 0$ we are in the state $|\psi_{3/2}\rangle$, describing a positive nucleus with $g$-factor $g_N$. The time evolution of the state is given by

$$|\psi_{3/2}(t)\rangle = \hat{U}(t)|\psi_{3/2}\rangle = e^{-i\hat{H}t/\hbar} |\psi_{3/2}\rangle = e^{-i\alpha t J_y} |\psi_{3/2}\rangle$$

where $\alpha = -g_N \mu_B B$.

Then the time evolution of $\langle \hat{J}_z \rangle$ is given by

$$\langle \hat{J}_z \rangle_t = \langle \psi_{3/2} | e^{i \alpha t J_y} \hat{J}_z e^{-i \alpha t J_y} | \psi_{3/2} \rangle |\psi\rangle$$

Now we have that

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

or

$$\hat{J}_x, \hat{J}_y = i\hat{J}_z, \quad \hat{J}_y, \hat{J}_z = i\hat{J}_x, \quad \hat{J}_z, \hat{J}_x = i\hat{J}_y$$

Thus,

$$e^{x \hat{J}_y \hat{J}_z e^{-x \hat{J}_y}} = \hat{J}_z + [\hat{J}_y, \hat{J}_z] x + [\hat{J}_y, [\hat{J}_y, \hat{J}_z]] \frac{x^2}{2} + [\hat{J}_y, [\hat{J}_y, [\hat{J}_y, \hat{J}_z]]] \frac{x^3}{6} + \ldots$$

$$e^{x \hat{J}_y \hat{J}_z e^{-x \hat{J}_y}} = \hat{J}_z + i\hat{J}_x x + [\hat{J}_y, i\hat{J}_x] \frac{x^2}{2} + [\hat{J}_y, [\hat{J}_y, i\hat{J}_x]] \frac{x^3}{6} + \ldots$$

$$e^{x \hat{J}_y \hat{J}_z e^{-x \hat{J}_y}} = \hat{J}_z + i\hat{J}_x x + [\hat{J}_y, i\hat{J}_x] \frac{x^2}{2} + [\hat{J}_y, [\hat{J}_y, i\hat{J}_x]] \frac{x^3}{6} + \ldots = \cos(\alpha t/\hbar) \hat{J}_z - \sin(\alpha t/\hbar) \hat{J}_x$$

where $x = i\alpha t/\hbar$. Therefore,

$$\langle \hat{J}_z \rangle_t = \langle \psi_{3/2} | \left( \cos(\alpha t) \hat{J}_z - \sin(\alpha t) \hat{J}_x \right) |\psi_{3/2}\rangle$$

$$= \cos(\alpha t) \langle \psi_{3/2} | \hat{J}_z |\psi_{3/2}\rangle - \sin(\alpha t) \langle \psi_{3/2} | \hat{J}_x |\psi_{3/2}\rangle$$

Now

$$\langle \psi_{3/2} | \hat{J}_z |\psi_{3/2}\rangle = 0$$

$$\langle \psi_{3/2} | \hat{J}_x |\psi_{3/2}\rangle = \frac{3\hbar}{2}$$

so that

$$\langle \hat{J}_z \rangle_t = \frac{3\hbar}{2} \sin g_N \mu_B B t$$

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 \( S_n = \hat{S} \cdot \hat{n} \) where the spin operator is
\[
\hat{S} = \hat{S}_x \hat{e}_x + \hat{S}_y \hat{e}_y + \hat{S}_z \hat{e}_z
\]
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
\[
|\hat{n}+\rangle = \cos \frac{\theta}{2} |z+\rangle + e^{i\varphi} \sin \frac{\theta}{2} |z-\rangle
\]
\[
|\hat{n}-\rangle = \sin \frac{\theta}{2} |z+\rangle - e^{i\varphi} \cos \frac{\theta}{2} |z-\rangle
\]
In the \( \hat{\sigma}_z \) basis we have
\[
\hat{S}_x = \frac{\hbar}{2} \hat{\sigma}_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}
\]
\[
\hat{S}_y = \frac{\hbar}{2} \hat{\sigma}_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}
\]
\[
\hat{S}_z = \frac{\hbar}{2} \hat{\sigma}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
\]
Therefore,
\[
\hat{S}_n = \hat{S} \cdot \hat{n} = (\hat{S}_x \hat{e}_x + \hat{S}_y \hat{e}_y + \hat{S}_z \hat{e}_z) \cdot (\sin \theta \cos \varphi \hat{e}_x + \sin \theta \sin \varphi \hat{e}_y + \cos \theta \hat{e}_z)
\]
\[
= \hat{S}_x \sin \theta \cos \varphi + \hat{S}_y \sin \theta \sin \varphi + \hat{S}_z \cos \theta = \frac{\hbar}{2} \begin{pmatrix} \cos \theta & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix}
\]
Eigenvalue/Eigenvector problem
\[
\hat{S}_n |\psi\rangle = \frac{\hbar}{2} |\psi\rangle
\]
or in matrix form
\[
\begin{pmatrix} \cos \theta & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix} \begin{pmatrix} \langle +\hat{z} | \psi\rangle \\ \langle -\hat{z} | \psi\rangle \end{pmatrix} = \lambda \begin{pmatrix} \langle +\hat{z} | \psi\rangle \\ \langle -\hat{z} | \psi\rangle \end{pmatrix}
\]
which is two homogeneous equations in two unknowns \( \langle \pm \hat{z} | \psi\rangle \). For a non-trivial solution, the determinant of the coefficients must vanish
\[
\begin{vmatrix} \cos \theta - \lambda & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta - \lambda \end{vmatrix} = 0 = -\cos^2 \theta - \sin^2 \theta + \lambda^2 \rightarrow \lambda^2 = 1 \rightarrow \lambda = \pm 1
\]
For \( \lambda = +1 \), we have
\[
\begin{pmatrix} \cos \theta & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix} \begin{pmatrix} \langle +\hat{z} | \psi\rangle \\ \langle -\hat{z} | \psi\rangle \end{pmatrix} = \begin{pmatrix} \langle +\hat{z} | \psi\rangle \\ \langle -\hat{z} | \psi\rangle \end{pmatrix}
\]
\[
(\cos \theta - 1) \langle +\hat{z} | \psi\rangle + e^{-i\varphi} \sin \theta \langle -\hat{z} | \psi\rangle = 0
\]
and from normalization

$$|\langle + \hat{z} | \psi \rangle|^2 + |\langle - \hat{z} | \psi \rangle|^2 = 1$$

so that

$$|\langle + \hat{z} | \psi \rangle|^2 \left[ 1 - \left( \frac{1 - \cos \theta}{\sin \theta} \right)^2 \right] = 1$$

$$|\langle + \hat{z} | \psi \rangle|^2 = \frac{(1 - \cos \theta)(1 + \cos \theta)}{2(1 - \cos \theta)} = \frac{(1 + \cos \theta)}{2} = \cos^2 \frac{\theta}{2}$$

and

$$\langle + \hat{z} | \psi \rangle = \cos \frac{\theta}{2}$$

$$\langle - \hat{z} | \psi \rangle = 1 - \cos \theta e^{-i\varphi} \sin \theta$$

Similarly, for \( \lambda = -1 \), we have

$$\begin{pmatrix} \cos \theta & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix} \begin{pmatrix} \langle + \hat{z} | \psi \rangle \\ \langle - \hat{z} | \psi \rangle \end{pmatrix} = - \begin{pmatrix} \langle + \hat{z} | \psi \rangle \\ \langle - \hat{z} | \psi \rangle \end{pmatrix}$$

and from normalization

$$|\langle + \hat{z} | \psi \rangle|^2 + |\langle - \hat{z} | \psi \rangle|^2 = 1$$

so that

$$|\langle + \hat{z} | \psi \rangle|^2 \left[ 1 + \left( \frac{1 + \cos \theta}{\sin \theta} \right)^2 \right] = 1$$

$$|\langle + \hat{z} | \psi \rangle|^2 = \frac{(1 + \cos \theta)(1 - \cos \theta)}{2(1 + \cos \theta)} = \frac{(1 - \cos \theta)}{2} = \sin^2 \frac{\theta}{2}$$

and

$$\langle - \hat{z} | \psi \rangle = -\frac{1 + \cos \theta}{e^{-i\varphi} \sin \theta} \langle + \hat{z} | \psi \rangle = -\frac{1 + \cos \theta}{e^{-i\varphi} \sin \theta} \sin \frac{\theta}{2}$$

$$= -\frac{1 + \cos \theta}{e^{-i\varphi} \sqrt{(1 - \cos \theta)(1 - \cos \theta)}} \sqrt{1 + \cos \theta} = -e^{-i\varphi} \cos \frac{\theta}{2}$$

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so that

\[ |\lambda = -1\rangle = (|+\hat{z}\rangle |\psi\rangle |+\hat{z}\rangle + (-|\hat{z}\rangle |\psi\rangle |-\hat{z}\rangle = \sin \frac{\theta}{2} |+\hat{z}\rangle - e^{i\varphi} \cos \frac{\theta}{2} |-\hat{z}\rangle = |-\hat{n}\rangle \]

**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 \( \theta \) 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 \( \theta \) in the \( x-z \) plane.

In the \( \hat{S}_z \) basis

\[
\hat{S}_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \rightarrow (\hat{S}_y)^2 = \frac{\hbar^2}{4} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{\hbar^2}{4} \hat{I}
\]

\[
\rightarrow (\hat{S}_y)^3 = \frac{\hbar^3}{8} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \frac{\hbar^3}{8} \hat{S}_y \rightarrow (\hat{S}_y)^4 = \frac{\hbar^4}{16} \hat{I} \quad \text{and so on} \ldots
\]

This implies that

\[
\hat{R}(\theta \hat{e}_y) = e^{-i \hat{S}_y \theta / \hbar} = \hat{I} + (\frac{-i \theta}{\hbar}) \hat{S}_y + \frac{1}{2!} (\frac{-i \theta}{\hbar})^2 (\hat{S}_y)^2 + \frac{1}{3!} (\frac{-i \theta}{\hbar})^3 (\hat{S}_y)^3 + \frac{1}{4!} (\frac{-i \theta}{\hbar})^4 (\hat{S}_y)^4 + \ldots
\]

\[
= \hat{I} + (\frac{-i \theta}{\hbar}) \sigma_y + \frac{1}{2!} (\frac{-i \theta}{\hbar})^2 (\frac{\hbar}{2})^2 \hat{I} + \frac{1}{3!} (\frac{-i \theta}{\hbar})^3 (\frac{\hbar}{2})^3 \sigma_y + \frac{1}{4!} (\frac{-i \theta}{\hbar})^4 (\frac{\hbar}{2})^4 \hat{I} + \ldots
\]

as expected from the general rule

\[
e^{-i \alpha \cdot \hat{n}} = \cos \alpha \hat{I} - i \hat{\sigma} \cdot \hat{n} \sin \alpha
\]

Therefore, converting to matrix form \( \hat{S}_z \) basis) we have

\[
\hat{R}(\theta \hat{e}_y) = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}
\]

so that

\[
\hat{R}(\theta \hat{e}_y) |+\hat{z}\rangle = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}
\]

\[
= \cos \frac{\theta}{2} |+\hat{z}\rangle + \sin \frac{\theta}{2} |-\hat{z}\rangle = |\hat{n}(\varphi = 0)\rangle
\]

and similarly for \(|\hat{n}(\varphi = 0)\rangle\).
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?

In the $\hat{\sigma}_z$ representation, the spin eigenvector is

$$|+\hat{z}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \hat{\sigma}_z |+\hat{z}\rangle = + |+\hat{z}\rangle \rightarrow \hat{S}_z |+\hat{z}\rangle = \frac{\hbar}{2} |+\hat{z}\rangle$$

The eigenvectors of $\hat{\sigma}_x$ in the $\hat{\sigma}_z$ representation are

$$|\pm\hat{x}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm1 \end{pmatrix} \rightarrow \hat{\sigma}_x |\pm\hat{x}\rangle = \pm |\pm\hat{x}\rangle$$

Expanding $|+\hat{z}\rangle$ in the $\hat{\sigma}_x$ states in the $\hat{\sigma}_z$ representation we have

$$|+\hat{z}\rangle = \frac{1}{\sqrt{2}} |+\hat{x}\rangle + \frac{1}{\sqrt{2}} |-\hat{x}\rangle$$

which says that the possible results of measuring $\hat{S}_x$ are $\pm\hbar/2$.

(b) What are the probabilities of finding these various results?

We have

$$P(+\hbar/2) = |\langle +\hat{x} | +\hat{z}\rangle|^2 = \frac{1}{2}$$

$$P(-\hbar/2) = |\langle -\hat{x} | +\hat{z}\rangle|^2 = \frac{1}{2}$$

so that

$$\langle \hat{S}_x \rangle = \frac{\hbar}{2} P(+\hbar/2) - \frac{\hbar}{2} P(-\hbar/2) = 0$$

(c) If the axis defining the measured spin direction makes an angle $\theta$ with respect to the original $z$-axis, what are the probabilities of various possible results?

Suppose that the spin axis is $\hat{n} = \hat{n}(\theta, \phi) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. Then the eigenfunctions for $\hat{S}_n = \hat{S} \cdot \hat{n}$ are (see earlier problem) in the $\hat{\sigma}_z$ basis are

$$|+\hat{n}\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} \end{pmatrix}, \quad |\pm\hat{n}\rangle = \begin{pmatrix} \sin \frac{\theta}{2} \\ -e^{i\phi} \cos \frac{\theta}{2} \end{pmatrix}$$

with eigenvalues $+\hbar/2$ and $-\hbar/2$ respectively.

Therefore

$$|+\hat{z}\rangle = \cos \frac{\theta}{2} |+\hat{n}\rangle + \sin \frac{\theta}{2} |-\hat{n}\rangle$$

so that

$$P(+\hbar/2; \hat{n}) = |\langle +\hat{n} | +\hat{z}\rangle|^2 = \cos^2 \frac{\theta}{2}$$

$$P(-\hbar/2; \hat{n}) = |\langle -\hat{n} | +\hat{z}\rangle|^2 = \sin^2 \frac{\theta}{2}$$
(d) What is the expectation value of the spin measurement in (c)?

\[ \langle \hat{S}_n \rangle = \frac{\hbar}{2} P(+\hbar/2) - \frac{\hbar}{2} P(-\hbar/2) = \frac{\hbar}{2} \left( \frac{\cos^2 \theta}{2} - \frac{\sin^2 \theta}{2} \right) = \frac{\hbar}{2} \cos \theta \]

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.

We have

\[ \hat{Q} = \frac{\hbar}{2} \hat{\sigma}_y + \frac{\hbar}{2} \hat{\sigma}_z \]

\[ \hat{Q}^2 = \frac{\hbar^2}{4} \left( A^2 \hat{\sigma}_y^2 + B^2 \hat{\sigma}_z^2 + AB \{ \hat{\sigma}_y, \hat{\sigma}_z \} \right) \]

\[ = \frac{\hbar^2}{4} \left( A^2 (1) + B^2 (1) + AB (0) \right) = \frac{\hbar^2}{4} (A^2 + B^2) \]

where we have used \( \hat{\sigma}_i^2 = \hat{I} \) and \( \{ \hat{\sigma}_i, \hat{\sigma}_j \} = 2 \delta_{ij} \hat{I} \). Therefore, the two eigenvalues of \( \hat{Q} \) are

\[ Q_{\pm} = \pm \frac{\hbar}{2} \sqrt{A^2 + B^2} \]

Alternatively, we could write in the \( \hat{S}_z \) basis

\[ \hat{Q} = \frac{\hbar}{2} \hat{\sigma}_y + \frac{\hbar}{2} \hat{\sigma}_z = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} B & -iA \\ iA & -B \end{pmatrix} \]

so that the characteristic equation is

\[ \begin{vmatrix} \frac{\hbar}{2} B - E & -i \frac{\hbar}{2} A \\ i \frac{\hbar}{2} A & -\frac{\hbar}{2} B - E \end{vmatrix} = 0 = \left( \left( \frac{\hbar B}{2} \right)^2 - E^2 \right) - \left( \frac{\hbar A}{2} \right)^2 \]

To get the eigenvectors we use

\[ \hat{Q} |\pm Q\rangle = \pm Q |\pm Q\rangle \rightarrow \frac{\hbar}{2} \begin{pmatrix} B & -iA \\ iA & -B \end{pmatrix} \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = \pm Q \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} \]

or

\[ \begin{align*}
\frac{\hbar}{2} B a_\pm - i \frac{\hbar}{2} A b_\pm &= Q_\pm a_\pm \\
i \frac{\hbar}{2} A a_\pm - \frac{\hbar}{2} B b_\pm &= Q_\pm b_\pm
\end{align*} \]
This gives
\[
\frac{b_{\pm}}{a_{\pm}} = \frac{2}{iA\hbar} \left( \frac{\hbar}{2} B - Q_{\pm} \right) = \frac{B}{iA} \mp \frac{1}{iA} \sqrt{A^2 + B^2}
\]
and
\[
\left( \begin{array}{c} a_{\pm} \\ b_{\pm} \end{array} \right) = N \left( \begin{array}{c} iA \\ B \mp \sqrt{A^2 + B^2} \end{array} \right) \text{ where } N = \text{ normalization factor}
\]

Normalizing, we find that
\[
\left( \begin{array}{c} a_{\pm} \\ b_{\pm} \end{array} \right) = \frac{1}{\sqrt{A^2 + (B \mp \sqrt{A^2 + B^2})^2}} \left( \begin{array}{c} iA \\ B \mp \sqrt{A^2 + B^2} \end{array} \right)
\]

(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 \(+\hbar/2\)?

In the \( \hat{S}_z \) basis we have
\[
|S_y = +\hbar/2\rangle = \frac{1}{\sqrt{2}} \left( \begin{array}{c} -i \\ 1 \end{array} \right)
\]

Therefore, the probability that \( S_y = +\hbar/2 \) in the states \( |\pm Q\rangle \) is given by
\[
P_{\pm}(S_y = +\hbar/2) = |\langle S_y = +\hbar/2 | \pm Q\rangle|^2
\]
\[
= \frac{1}{\sqrt{2}} \left( \begin{array}{c} -i \\ 1 \end{array} \right) \cdot \left( \begin{array}{c} a_{\pm} \\ b_{\pm} \end{array} \right) = \frac{1}{2} |a_{\pm} + b_{\pm}|^2
\]
\[
= \frac{1}{2} \left( |a_{\pm}|^2 + |b_{\pm}|^2 - ia_{\pm}^* b_{\pm} + ia_{\pm} b_{\pm}^* \right) = \frac{1}{2} \left( 1 - ia_{\pm}^* b_{\pm} + ia_{\pm} b_{\pm}^* \right)
\]
or
\[
P_{\pm}(S_y = +\hbar/2) = \frac{1}{2} \left( 1 - \frac{2A (B \mp \sqrt{A^2 + B^2})}{A^2 + (B \mp \sqrt{A^2 + B^2})^2} \right)
\]

9.7.12 Simultaneous Measurement

A beam of particles is subject to a simultaneous measurement of the angular momentum observables \( \hat{L}_z \) and \( \hat{L}_y \). The measurement gives pairs of values
\[
(\ell, m) = (0, 0) \text{ and } (1, -1)
\]
with probabilities 3/4 and 1/4 respectively.
(a) Reconstruct the state of the beam immediately before the measurements.

The state of the beam is, in terms of the eigenstates of $L_z$,

$$|\psi\rangle = \frac{\sqrt{3}}{2} |0, 0\rangle + \frac{1}{2} e^{i\alpha} |1, -1\rangle$$

where $\alpha$ is an arbitrary phase.

(b) The particles in the beam with $(\ell, m) = (1, -1)$ are separated out and subjected to a measurement of $L_x$. What are the possible outcomes and their probabilities?

The possible outcomes will correspond to the common eigenvectors of $L^2$, $L_z$,

$$|1, m_x = 1\rangle , |1, m_x = 0\rangle , |1, m_x = -1\rangle$$

Each of these can be expanded in terms of $L_z$ eigenstates:

$$|1, m_x\rangle = C_1 |1, 1\rangle + C_0 |1, 0\rangle + C_{-1} |1, -1\rangle$$

Acting on this state with

$$L_x = (L_+ + L_-)/2$$

we should get $m_x \hbar$. Doing this, we obtain the following relations between the coefficients

$$C_0 = m_x \sqrt{2} C_1 = m_x \sqrt{2} C_{-1} , \quad C_1 + C_{-1} = m_x \sqrt{2} C_0$$

Therefore, we are led to

$$|1, m_x = 1\rangle = \frac{1}{2} \left( |1, 1\rangle + \sqrt{2} |1, 0\rangle + |1, -1\rangle \right)$$

$$|1, m_x = 0\rangle = \frac{1}{\sqrt{2}} \left( |1, 1\rangle - |1, -1\rangle \right)$$

$$|1, m_x = -1\rangle = \frac{1}{2} \left( |1, 1\rangle - \sqrt{2} |1, 0\rangle + |1, -1\rangle \right)$$

The inverse expression for the $L_z$ eigenstates are

$$|1, 1\rangle = \frac{1}{\sqrt{2}} |1, m_x = 1\rangle + \frac{1}{2} |1, m_x = 0\rangle + |1, m_x = -1\rangle$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}} |1, m_x = 1\rangle - \frac{1}{\sqrt{2}} |1, m_x = -1\rangle$$

$$|1, -1\rangle = -\frac{1}{\sqrt{2}} |1, m_x = 1\rangle + \frac{1}{2} |1, m_x = 0\rangle + |1, m_x = -1\rangle$$

From these states we can read off the probabilities:

$$P_{L_z = \pm \hbar} = \frac{1}{4} , \quad P_{L_z = 0} = \frac{1}{2}$$

(c) Construct the spatial wave functions of the states that could arise from the second measurement.

Using the standard formulas for the spherical harmonics we obtain for the eigenfunctions of $L_x$

$$\psi_{\pm 1} = \sqrt{\frac{3}{8\pi}} \left( \pm \cos \theta - i \sin \varphi \sin \theta \right) , \quad \psi_0 = -\sqrt{\frac{3}{4\pi}} \cos \varphi \sin \theta$$

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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 $\varphi$, 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.

Consider the operator

$$X_i = e^{-i\varphi L_x/\hbar} V_i e^{i\varphi L_x/\hbar}$$

as a function of $\varphi$ and differentiate it with respect to $\varphi$. We get

$$\frac{dX_i}{d\varphi} = \epsilon_{xij} X_j$$

From this we obtain

$$\frac{dX_x}{d\varphi} = \epsilon_{xxy} X_y = 0 \Rightarrow X_x(\varphi) = X_x(0) = V_x$$
$$\frac{dX_x}{d\varphi} = \epsilon_{xxy} X_y = X_z$$
$$\frac{dX_z}{d\varphi} = \epsilon_{zzj} X_j = -X_y$$

The last two equations give

$$\frac{d^2X_y}{d\varphi^2} = -X_y \Rightarrow X_y(\varphi) = X_y(0) \cos \varphi + X_z(0) \sin \varphi = V_y \cos \varphi + V_z \sin \varphi$$
$$\frac{d^2X_z}{d\varphi^2} = -X_z \Rightarrow X_z(\varphi) = X_z(0) \cos \varphi - X_y(0) \sin \varphi = V_z \cos \varphi - V_y \sin \varphi$$

or

$$e^{-i\varphi L_x/\hbar} V_i e^{i\varphi L_x/\hbar} = \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & \cos \varphi & \sin \varphi \\ 0 & -\sin \varphi & \cos \varphi \end{array}\right)\left(\begin{array}{c} V_x \\ V_y \\ V_z \end{array}\right) = R_{ij} V_j$$

where the matrix $R$ is a rotation matrix corresponding to a rotation around the $x$–axis by an angle $\varphi$. 
(b) Prove that
\[ e^{-i\varphi L_x} |\ell, m\rangle = |\ell, -m\rangle \]
Putting \( \varphi = \pi \) in the expression from (a) we get
\[ e^{-i\varphi L_x/h} L_x e^{i\varphi L_x/h} = R_{z_j} L_j = R_{z \ell} L_z = -L_z \]
Acting on the rotated state with \( L_z \) we get
\[ L_z e^{i\pi L_x/h} |\ell, m\rangle = -e^{-i\pi L_x/h} L_z |\ell, m\rangle = -\hbar m e^{-i\pi L_x/h} |\ell, m\rangle \]
Thus,
\[ e^{i\pi L_x/h} |\ell, m\rangle = |\ell, -m\rangle \]

(c) Show that a rotation by \( \pi \) 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 \( \pi \) and, finally rotating back by \( -\pi/2 \) around the \( x \)-axis. In terms of rotation operators this is expressed by
\[ e^{i\pi L_x/2\hbar} e^{-i\pi L_y/\hbar} e^{-i\pi L_x/2\hbar} = e^{-i\pi L_z/\hbar} \]
Putting \( \varphi = \pi/2 \) in the rotation matrix, we get
\[ e^{-i\pi L_x/2\hbar} \begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} e^{i\pi L_x/2\hbar} = \begin{pmatrix} L_x \\ L_z \\ -L_y \end{pmatrix} \]
Thus, we obtain
\[ e^{-i\pi L_x/2\hbar} (L_y)^n e^{i\pi L_x/2\hbar} e^{-i\pi L_y/\hbar} e^{i\pi L_x/2\hbar} \ldots \ldots = (L_z)^n \]
and finally
\[ e^{-i\pi L_x/2\hbar} e^{-i\pi L_y/\hbar} e^{i\pi L_x/2\hbar} = e^{-i\pi L_z/\hbar} \]

9.7.14 Addition of Angular Momentum

Two atoms with \( J_1 = 1 \) and \( J_2 = 2 \) are coupled, with an energy described by
\[ \hat{H} = \varepsilon \hat{J}_1 \cdot \hat{J}_2, \varepsilon > 0. \]
Determine all of the energies and degeneracies for the coupled system.

We have
\[ \hat{J} = \hat{J}_1 + \hat{J}_2 \Rightarrow \hat{J} \cdot \hat{J} = \frac{1}{2} \left( \hat{J}_1^2 - \hat{J}_1^2 - \hat{J}_2^2 \right) \]
\[ = \frac{1}{2} \left( \hat{J}_1^2 - \hbar^2 J_1(J_1 + 1)I - \hbar^2 J_2(J_2 + 1)I \right) \]
\[ = \frac{1}{2} \left( \hbar^2 J(J + 1)I - 2\hbar^2 \hat{I} - 6\hbar^2 \hat{I} \right) \]
\[ = \frac{\hbar^2}{2} J(J + 1) - 8 \hat{I} \]
when acting on a \(|J, M\rangle\) state. The energies depend only on \(J\) and hence are \(2J + 1\) degenerate (\(M\) values).

Now the possible values of \(J\) are given by

\[ J = J_1 + J_2, \ldots, |J_1 - J_2| = 3, 2, 1 \]

Thus, the final configurations are

\begin{align*}
J = 1 & : |1, 1\rangle, |1, 0\rangle, |1, -1\rangle \Rightarrow E = -3\varepsilon \hbar^2 \\
J = 2 & : |2, 2\rangle, |2, 1\rangle, |2, 0\rangle, |2, -1\rangle, |2, -2\rangle \Rightarrow E = -\varepsilon \hbar^2 \\
J = 3 & : |3, 3\rangle, |3, 2\rangle, |3, 1\rangle, |3, 0\rangle, |3, -1\rangle, |3, -2\rangle, |3, -3\rangle \Rightarrow E = 2\varepsilon \hbar^2
\end{align*}

### 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 \((3 \times 3)\) of the angular momentum operators \(\hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{S}^2, \hat{S}_+, \) and \(\hat{S}_-\). In the \(|1, 1\rangle, |1, 0\rangle\) and \(|1, -1\rangle\) or \(|\hat{S}, \hat{S}_z\rangle\) basis the \(\hat{S}_z\) operator is diagonal (by definition)

\[ \hat{S}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \]

Now using

\[ \hat{S}_\pm |s, m\rangle = \hbar \sqrt{s(s + 1) - m(m \pm 1)} |s, m \pm 1\rangle \]

in the \(s = 1\) basis we have

\[ \hat{S}_+ = \begin{pmatrix} \langle 1, 1| \hat{S}_+ |1, 1\rangle & \langle 1, 1| \hat{S}_+ |1, 0\rangle & \langle 1, 1| \hat{S}_+ |1, -1\rangle \\ \langle 1, 0| \hat{S}_+ |1, 1\rangle & \langle 1, 0| \hat{S}_+ |1, 0\rangle & \langle 1, 0| \hat{S}_+ |1, -1\rangle \\ \langle 1, -1| \hat{S}_+ |1, 1\rangle & \langle 1, -1| \hat{S}_+ |1, 0\rangle & \langle 1, -1| \hat{S}_+ |1, -1\rangle \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{2}\hbar & 0 \\ 0 & 0 & \sqrt{2}\hbar \\ 0 & 0 & 0 \end{pmatrix} = \sqrt{2}\hbar \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \]

Therefore,

\[ \hat{S}_- = \hat{S}_+^\dagger = \sqrt{2}\hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

and

\[ \hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} \]

\[ \hat{S}_y = \frac{\hat{S}_+ - \hat{S}_-}{2i} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \]

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Finally,
\[
\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2
\]
\[
= \frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} + \frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix} + \hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]
\[
= 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = 1(1+1)\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]
(b) Determine the eigenstates of \(\hat{S}_x\) in terms of the eigenstates \(|1,1\rangle, |1,0\rangle\) and \(|1,-1\rangle\) of \(\hat{S}_z\).

We have the eigenvalue/eigenvector equation \(\hat{S}_x |1,m\rangle_x = m\hbar |1,m\rangle_x\), or in matrix form
\[
\frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = m\hbar \begin{pmatrix} a \\ b \\ c \end{pmatrix}
\]
For a non-trivial solution, we must have
\[
\begin{vmatrix}
-\frac{m}{\sqrt{2}} & \frac{\sqrt{2}}{2} & 0 \\
\frac{\sqrt{2}}{2} & -m & \frac{\sqrt{2}}{2} \\
0 & \frac{\sqrt{2}}{2} & -m \\
\end{vmatrix} = 0 = -m^3 + m \rightarrow m = 0, \pm 1
\]
as expected. Substituting \(m = 1\) into the eigenvalue equation, we get
\[
\frac{\sqrt{2}}{2} b = a , \quad \frac{\sqrt{2}}{2} (a + c) = b , \quad \frac{\sqrt{2}}{2} b = c
\]
so that
\[
a = c , \quad b = \sqrt{2} a
\]
\[
\rightarrow |1,1\rangle_x = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2} |1,1\rangle + \frac{\sqrt{2}}{2} |1,0\rangle + \frac{1}{2} |1,-1\rangle
\]
In a similar manner, we have for \(m = 0\)
\[
b = 0 , \quad a + c = 0
\]
\[
\rightarrow |1,0\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} |1,1\rangle - \frac{1}{\sqrt{2}} |1,-1\rangle
\]
and for \(m = -1\)
\[
\frac{\sqrt{2}}{2} b = -a , \quad \frac{\sqrt{2}}{2} (a + c) = -b , \quad \frac{\sqrt{2}}{2} b = -c
\]
\[
|1,-1\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2} |1,1\rangle - \frac{\sqrt{2}}{2} |1,0\rangle + \frac{1}{2} |1,-1\rangle
\]
(c) A spin = 1 particle is in the state
\[ |\psi\rangle = \frac{1}{\sqrt{14}} \left( \begin{array}{c}
1 \\
2 \\
3i
\end{array} \right) \]
in the \( \hat{S}_z \) basis.

\[ |\psi\rangle = \left( \begin{array}{c}
\langle 1, 1 | \psi \rangle \\
\langle 1, 0 | \psi \rangle \\
\langle 1, -1 | \psi \rangle
\end{array} \right) = \frac{1}{\sqrt{14}} \left( \begin{array}{c}
1 \\
2 \\
3i
\end{array} \right) \text{ in the } \hat{S}_z \text{ basis} \]

(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 \( \langle \hat{S}_z \rangle \)?

\[
P(S_z = +\hbar) = |\langle 1, 1 | \psi \rangle|^2 = \left| \frac{1}{\sqrt{14}} \right|^2 = \frac{1}{14}
\]
\[
P(S_z = 0) = |\langle 1, 0 | \psi \rangle|^2 = \left| \frac{2}{\sqrt{14}} \right|^2 = \frac{2}{7}
\]
\[
P(S_z = -\hbar) = |\langle 1, -1 | \psi \rangle|^2 = \left| \frac{3i}{\sqrt{14}} \right|^2 = \frac{9}{14}
\]

\[
\langle S_z \rangle = \sum_{S_z} S_z P(S_z) = \hbar \left( \frac{1}{14} \right) + 0 \left( \frac{2}{7} \right) - \hbar \left( \frac{9}{14} \right) = -\frac{4}{7} \hbar
\]

(2) What is \( \langle \hat{S}_x \rangle \) in this state?

\[
\langle S_x \rangle = \langle \psi | \hat{S}_x | \psi \rangle = \frac{1}{\sqrt{14}} (1, 2, -3i) \frac{\hbar}{\sqrt{2}} \left( \begin{array}{ccc}
0 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0
\end{array} \right) \frac{1}{\sqrt{14}} \left( \begin{array}{c}
1 \\
2 \\
3i
\end{array} \right) = \frac{\sqrt{2}}{7} \hbar
\]

(3) What is the probability that a measurement of \( \hat{S}_x \) will yield the value \( \hbar \) for this state?

\[
|1, 1 \rangle_x = \frac{1}{2} \left( \begin{array}{c}
1 \\
\sqrt{2}
\end{array} \right) = \frac{1}{2} |1, 1 \rangle + \frac{\sqrt{2}}{2} |1, 0 \rangle + \frac{1}{2} |1, -1 \rangle
\]

Therefore,

\[
x \langle 1, 1 | \psi \rangle = \left( \frac{1}{2} \langle 1, 1 | + \frac{\sqrt{2}}{2} \langle 1, 0 | + \frac{1}{2} \langle 1, -1 | \right) \frac{1}{\sqrt{14}} (|1, 1 \rangle + 2 |1, 0 \rangle + 3i |1, -1 \rangle)
\]
\[
= \frac{1}{2} \frac{1}{\sqrt{14}} (1 + 2\sqrt{2} + 3i)
\]

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and
\[ P(S_x = +\hbar) = |\langle 1, 1 | \psi \rangle|^2 = \left| \frac{1}{2 \sqrt{14}} (1 + 2\sqrt{2} + 3i) \right|^2 \]
\[ = \frac{1}{56} (1 + 4\sqrt{2} + 8 + 9) = \frac{1}{28} (9 + 2\sqrt{2}) \]

(d) A particle with spin = 1 has the Hamiltonian
\[ \hat{H} = A\hat{S}_z + \frac{B}{\hbar}\hat{S}^2 \]

(1) Calculate the energy levels of this system.

Using (a) we have
\[ \hat{H} = \hbar \begin{pmatrix} A + B/2 & 0 & B/2 \\ 0 & B & 0 \\ B/2 & 0 & -A + B/2 \end{pmatrix} \]

The characteristic equation determines the eigenvalues
\[ \begin{vmatrix} Ah + Bh/2 - E & 0 & Bh/2 \\ 0 & Bh - E & 0 \\ Bh/2 & 0 & -Ah + Bh/2 - E \end{vmatrix} = 0 \]
or
\[ (Bh - E) (Ah + Bh/2 - E) (-Ah + Bh/2 - E) - (Bh - E) (Bh/2) (Bh/2) = 0 \]
\[ (Bh - E) (Bh/2 - E)^2 - (Ah)^2 - (Bh/2)^2 = 0 \]
so that
\[ E_0 = \hbar B \; , \; E_{\pm} = \frac{B}{2} \pm \sqrt{\hbar^2 A^2 + \frac{\hbar^2 B^2}{4}} \]

We now determine the eigenvectors.

For \( E_0 = \hbar B = B' \)
\[ \hbar \begin{pmatrix} A + B/2 & 0 & B/2 \\ 0 & B & 0 \\ B/2 & 0 & -A + B/2 \end{pmatrix} \begin{pmatrix} a_0 \\ b_0 \\ c_0 \end{pmatrix} = \hbar B \begin{pmatrix} a_0 \\ b_0 \\ c_0 \end{pmatrix} \]
\[ \rightarrow a_0 = c_0 = 0 \; , \; b_0 = 1 \rightarrow |E_0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \]

For \( E_+ = \frac{\hbar}{2} (B + \sqrt{4A^2 + B^2}) \)
\[ \hbar \begin{pmatrix} A + B/2 & 0 & B/2 \\ 0 & B & 0 \\ B/2 & 0 & -A + B/2 \end{pmatrix} \begin{pmatrix} a_+ \\ b_+ \\ c_+ \end{pmatrix} = \lambda_+ \hbar \begin{pmatrix} a_+ \\ b_+ \\ c_+ \end{pmatrix} \]
\[ = \frac{\hbar}{2} \left( B + \sqrt{4A^2 + B^2} \right) \begin{pmatrix} a_+ \\ b_+ \\ c_+ \end{pmatrix} \]

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\[ (A + \frac{B}{2}) a_+ + \frac{B}{2} c_+ = \lambda_a a_+ \]
\[ B b_+ = \lambda_b b_+ \rightarrow b_+ = 0 \]
\[ \frac{B}{2} a_+ + (-A + \frac{B}{2}) c_+ = \lambda_c c_+ \]
\[ a_+^2 + c_+^2 = 1 \]

Then,
\[ \frac{a_+}{c_+} = -\frac{\frac{B}{2}}{A + \frac{B}{2} - \lambda_+} = -\frac{B}{2A - \sqrt{4A^2 + B^2}} = -\frac{B}{2A - \omega} , \quad \omega = \sqrt{4A^2 + B^2} \]
\[ a_+^2 + c_+^2 = 1 \rightarrow \begin{cases} \lambda_a = \frac{B}{\sqrt{B^2 + (\omega - 2A)^2}} , & \omega = \frac{\omega - 2A}{\sqrt{B^2 + (\omega - 2A)^2}} \\
\end{cases} \]
\[ \rightarrow |E_+\rangle = \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} \begin{pmatrix} B \\ 0 \end{pmatrix} \]

Using orthonormality, we then have
\[ |E_-\rangle = \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} \begin{pmatrix} \omega - 2A \\ 0 \\ -B \end{pmatrix} \]

(2) If, at \( t = 0 \), the system is in an eigenstate of \( \hat{S}_z \) with eigenvalue \( \hbar \), calculate the expectation value of the spin \( \langle \hat{S}_Z \rangle \) at time \( t \).

Now
\[ |\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle \]

and
\[ |\psi(0)\rangle = |S_z = +\hbar\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} (B |E_+\rangle + (\omega - 2A) |E_-\rangle) \]

so that
\[ |\psi(t)\rangle = \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} \left( B e^{-i\hat{H}t/\hbar} |E_+\rangle + (\omega - 2A) e^{-i\hat{H}t/\hbar} |E_-\rangle \right) \]
\[ = \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} \left( B e^{-i\hat{E}_+ t/\hbar} |E_+\rangle + (\omega - 2A) e^{-i\hat{E}_- t/\hbar} |E_-\rangle \right) \]

Now
\[ \hat{S}_z |E_+\rangle = \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} \begin{pmatrix} B \\ 0 \\ -(\omega - 2A) \end{pmatrix} \]
\[ \hat{S}_z |E_-\rangle = \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} \begin{pmatrix} 0 \\ B \\ (\omega - 2A) \end{pmatrix} \]
Thus,

\[
\langle S_z \rangle_t = \langle \psi(t) | \hat{S}_z | \psi(t) \rangle
\]

\[
= \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} \left( \frac{B e^{iE_+ t/\hbar} (E_+) + (\omega - 2A) e^{iE_- t/\hbar} (E_-)}{B e^{-iE_+ t/\hbar} \begin{pmatrix} B \\ 0 \\ -(\omega - 2A) \end{pmatrix} + (\omega - 2A) e^{-iE_- t/\hbar} \begin{pmatrix} (\omega - 2A) \\ 0 \\ B \end{pmatrix}} \right)
\]

After lots of algebra, we find

\[
\langle S_z \rangle_t = \frac{1}{(B^2 + (\omega - 2A)^2)^2} \left( (B^2 + (\omega - 2A)^2)^2 + 4B^2(\omega - 2A)^2 \cos \left( \frac{E_+ - E_-}{\hbar} \right) \right)
\]

Some limits:

(a) Let \( B \to 0, \ \omega \to 2A. \) We find \( \langle S_z \rangle_t = \hbar = \text{constant since} \)

\[
\left[ \hat{\mathcal{H}}(B = 0), \hat{S}_z \right] = 0
\]

(b) Let \( A \to 0, \ \omega \to B. \) We find

\[
\langle S_z \rangle_t = \hbar \cos \left( \frac{E_+ - E_-}{\hbar} \right) = \hbar \cos \left( \frac{hB - 0}{\hbar} \right) = \hbar \cos (Bt)
\]

which corresponds to precession.

### 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 \( J^2 \) and \( F^2 \) are \( J(J + 1)h^2 \) and \( F(F + 1)h^2 \) 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?

For the 1s ground state we have

\[
L = 0 \Rightarrow \vec{J} = \vec{L} + \vec{S} = \vec{S} \Rightarrow J = S = 1/2
\]

Since \( \vec{F} = \vec{J} + \vec{I} \) and \( I = 1 \), the possible values of \( F \) are

\[
F = J + I, \ldots, |J - I| = 3/2, 1/2
\]
(b) What are the possible values of the quantum numbers $J$ and $F$ for a deuterium atom in the $2p(L = 1)$ excited state?

For the $2p$ excited state, we have $L = 1$. The possible values for $J$ are

$$J = L + S, ...., |L - S| = 3/2, 1/2$$

The possible values for $F$ are

$$F = J + I, ...., |J - I|$$

For $J = 3/2$ we have

$$F = 5/2, 3/2, 1/2$$

For $J = 1/2$ we have

$$F = 3/2, 1/2$$

So the possible values of $F$ are

$$F = 5/2, 3/2, 1/2$$

**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 $Y_{1}^{\pm 1,0}$ functions in terms of $x, y, z$ and $r$ that

$$Y_{1}^{\pm 1} = \left(\frac{3}{4\pi}\right)^{1/2} \frac{x \pm iy}{\sqrt{2r}}, \quad Y_{1}^{0} = \left(\frac{3}{4\pi}\right)^{1/2} \frac{z}{r}$$

$$Y_{1}^{\pm 1} = \pm \frac{3}{8\pi} e^{\pm i\phi} \sin \theta = \pm \sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$$

$$Y_{1}^{0} = \sqrt{\frac{3}{4\pi}} \cos \theta = \sqrt{\frac{3}{8\pi}} \frac{z}{r}$$

or

$$Y_{1}^{0} - Y_{1}^{+1} = 2i \sqrt{\frac{3}{8\pi}} \frac{y}{r}$$

$$-Y_{1}^{-1} + Y_{1}^{+1} = 2 \sqrt{\frac{3}{8\pi}} \frac{x}{r}$$

(b) Using this result, show that for a particle described by $\psi$ above

$$P(L_z = 0) = 2/3, \quad P(L_z = \hbar) = 1/6, \quad P(L_z = -\hbar) = 1/6$$

Thus, we have

$$\psi = N(x + y + 2z)e^{-\alpha r} = Nf(r) \left(\frac{1 + i}{\sqrt{2}} Y_{1}^{-1} - \frac{1 - i}{\sqrt{2}} Y_{1}^{+1} + 2Y_{1}^{0}\right)$$

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or
\[ |\psi\rangle = \frac{1}{\sqrt{6}} \left( \frac{1+i}{\sqrt{2}} |1, -1\rangle - \frac{1-i}{\sqrt{2}} |1, 1\rangle + 2 |1, 0\rangle \right) \]

Therefore,
\[
\begin{align*}
P(L_z = 0 | \psi) &= |\langle 1, 0 | \psi \rangle|^2 = \frac{1}{6} \left| \frac{1+i}{\sqrt{2}} \right|^2 = \frac{1}{6} \\
P(L_z = +1 | \psi) &= |\langle 1, 1 | \psi \rangle|^2 = \frac{1}{6} \left| \frac{1-i}{\sqrt{2}} \right|^2 = \frac{1}{6} \\
P(L_z = -1 | \psi) &= |\langle -1, -1 | \psi \rangle|^2 = \frac{1}{6} \left( \frac{1}{3} \right) = \frac{2}{3}
\end{align*}
\]

### 9.7.18 Spin in Magnetic Field

Suppose that we have a spin–1/2 particle interacting with a magnetic field via the Hamiltonian
\[
\hat{H} = \begin{cases} 
-\vec{\mu} \cdot \vec{B}, & \vec{B} = B\hat{e}_z \quad 0 \leq t < T \\
-\vec{\mu} \cdot \vec{B}, & \vec{B} = B\hat{e}_y \quad T \leq t < 2T
\end{cases}
\]

where \(\vec{\mu} = \mu_B \vec{\sigma}\) and the system is initially \((t = 0)\) in the state
\[ |\psi(0)\rangle = |x\rangle = \frac{1}{\sqrt{2}} (|z\rangle + |z\rangle) \]

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)

During the time interval \(0 \leq t < T\) we have
\[ \hat{H} = -\hbar \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

so that the Schrodinger equation becomes
\[
\begin{align*}
\hbar \frac{\partial}{\partial t} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} &= i\hbar \begin{pmatrix} \dot{\alpha} \\ \dot{\beta} \end{pmatrix} = \hat{H} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -\hbar \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -\hbar \omega \begin{pmatrix} \alpha \\ -\beta \end{pmatrix}
\end{align*}
\]

or
\[
\begin{align*}
\dot{\alpha} &= i\omega \alpha \rightarrow \alpha(t) = Ae^{i\omega t} \\
\dot{\beta} &= -i\omega \beta \rightarrow \beta(t) = Be^{-i\omega t}
\end{align*}
\]

The initial state \((t = 0)\) is
\[ |\psi(0)\rangle = |x\rangle = \frac{1}{\sqrt{2}} (|z\rangle + |z\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \]

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so that
\[ \alpha(0) = \frac{1}{\sqrt{2}} = A, \quad \beta(0) = \frac{1}{\sqrt{2}} = B \]
and
\[ |\psi(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega t} \\
- e^{-i\omega t} \end{pmatrix} \rightarrow |\psi(T)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega T} \\
- e^{-i\omega T} \end{pmatrix} \]
Now during the time interval \( T \leq t \leq 2T \) we have
\[ \hat{H} = -\hbar \omega \begin{pmatrix} 0 & -i \\
i & 0 \end{pmatrix} \]
so that the Schrodinger equation becomes
\[ i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \alpha \\
\beta \end{pmatrix} = i\hbar \begin{pmatrix} \dot{\alpha} \\
\dot{\beta} \end{pmatrix} = \hat{H} \begin{pmatrix} \alpha \\
\beta \end{pmatrix} = -\hbar \omega \begin{pmatrix} 0 & -i \\
i & 0 \end{pmatrix} \begin{pmatrix} \alpha \\
\beta \end{pmatrix} = -i\hbar \omega \begin{pmatrix} -\beta \\
\alpha \end{pmatrix} \]
or
\[ \dot{\alpha} = \omega \beta \rightarrow \dot{\alpha} = \omega \dot{\beta} = -\omega^2 \alpha \rightarrow \alpha(t) = c_1 e^{i\omega t} + c_2 e^{-i\omega t} \]
\[ \dot{\beta} = -\omega \alpha \rightarrow \dot{\beta} = -\omega \dot{\alpha} = -\omega^2 \beta \rightarrow \beta(t) = c_3 e^{i\omega t} + c_4 e^{-i\omega t} \]
Now
\[ \dot{\alpha} = \omega \beta \rightarrow ic_1 = c_3, \quad -ic_2 = c_4 \]
\[ \dot{\beta} = -\omega \alpha \rightarrow ic_3 = -c_1, \quad -ic_4 = -c_2 \]
so that
\[ c_3 = ic_1 \text{ and } c_4 = -ic_2 \]
and
\[ \alpha(t) = c_1 e^{i\omega t} + c_2 e^{-i\omega t} \]
\[ \beta(t) = i(c_1 e^{i\omega t} - c_2 e^{-i\omega t}) \]
The initial state (at \( t = T \)) is
\[ |\psi(T)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega T} \\
n- e^{-i\omega T} \end{pmatrix} \]
so that
\[ \alpha(T) = c_1 e^{i\omega T} + c_2 e^{-i\omega T} = \frac{1}{\sqrt{2}} e^{i\omega T} \]
\[ \beta(T) = i(c_1 e^{i\omega T} - c_2 e^{-i\omega T}) = \frac{1}{\sqrt{2}} e^{-i\omega T} \]
or
\[ c_1 e^{i\omega T} + c_2 e^{-i\omega T} = \frac{1}{\sqrt{2}} e^{i\omega T} \]
\[ c_1 e^{i\omega T} - c_2 e^{-i\omega T} = -\frac{i}{\sqrt{2}} e^{-i\omega T} \]
and
\[ 2c_1 e^{i\omega T} = \frac{1}{\sqrt{2}} (e^{i\omega T} - ie^{-i\omega T}) \]
\[ 2c_2 e^{-i\omega T} = \frac{1}{\sqrt{2}} (e^{i\omega T} + ie^{-i\omega T}) \]

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Finally, for $T \leq t \leq 2T$

$$|\psi(t)\rangle = \left( \begin{array}{c} \alpha(t) \\ \beta(t) \end{array} \right) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} c_1 e^{i\omega t} + c_2 e^{-i\omega t} \\ ic_1 e^{i\omega t} - c_2 e^{-i\omega t} \end{array} \right)$$

$$= \left( \begin{array}{c} \frac{1}{\sqrt{2}} e^{-i\omega T} (e^{i\omega T} - ie^{-i\omega T}) e^{i\omega t} + \left( \frac{1}{2\sqrt{2}} e^{i\omega T} (e^{i\omega T} + ie^{-i\omega T}) \right) e^{-i\omega t} \\ \frac{1}{2\sqrt{2}} e^{-i\omega T} (e^{i\omega T} - ie^{-i\omega T}) e^{i\omega t} - \left( \frac{1}{2\sqrt{2}} e^{i\omega T} (e^{i\omega T} + ie^{-i\omega T}) \right) e^{-i\omega t} \end{array} \right)$$

Now, we need

$$\langle S_x = + | \psi(2T) \rangle$$

$$= \frac{1}{\sqrt{2}} \langle 1, 1 \rangle \left( \begin{array}{c} \left( \frac{1}{2\sqrt{2}} e^{-i\omega T} (e^{i\omega T} - ie^{-i\omega T}) \right) e^{2i\omega T} + \left( \frac{1}{2\sqrt{2}} e^{i\omega T} (e^{i\omega T} + ie^{-i\omega T}) \right) e^{-2i\omega T} \\ \left( \frac{1}{2\sqrt{2}} e^{-i\omega T} (e^{i\omega T} - ie^{-i\omega T}) \right) e^{2i\omega T} - \left( \frac{1}{2\sqrt{2}} e^{i\omega T} (e^{i\omega T} + ie^{-i\omega T}) \right) e^{-2i\omega T} \end{array} \right)$$

$$= \frac{1}{4} ((e^{2i\omega T} - i) + (1 + ie^{-2i\omega T}) + i (e^{2i\omega T} - i) - i (1 + ie^{-2i\omega T}))$$

$$= \frac{1}{4} ((1 + i)(e^{2i\omega T} + e^{-2i\omega T}) + 2(1 - i))$$

so that

$$\text{Prob} = \frac{1}{16} \left( (2 + 2 \cos 2\omega T)^2 + (2 - 2 \cos 2\omega T)^2 \right)$$

$$= \frac{1}{16} (8 + 8 \cos^2 2\omega T) = \frac{1}{2} (1 + \cos^2 2\omega T)$$

(2) Using the time development operator (using operator algebra)

During the time interval $0 \leq t < T$ we have

$$\hat{H} = -\hbar \omega \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right)$$

The eigenvectors and eigenvalues of $\hat{H}$ are

$$|z+\rangle = \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \rightarrow E_+ = -\hbar \omega \quad , \quad |z-\rangle = \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \rightarrow E_- = +\hbar \omega$$

Initially,

$$|\psi(0)\rangle = |x+) = \frac{1}{\sqrt{2}} (|z+\rangle + |z-\rangle) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ 1 \end{array} \right)$$

Therefore,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = e^{-i\hat{H}t/\hbar} \frac{1}{\sqrt{2}} (|z+\rangle + |z-\rangle) = \frac{1}{\sqrt{2}} (e^{i\omega t} |z+\rangle + e^{-i\omega t} |z-\rangle)$$

so that

$$|\psi(T)\rangle = \frac{1}{\sqrt{2}} (e^{i\omega T} |z+\rangle + e^{-i\omega T} |z-\rangle) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} e^{i\omega T} \\ e^{-i\omega T} \end{array} \right)$$
as in part (1).

Now during the time interval $T \leq t \leq 2T$ we have

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

$$|\psi(T)\rangle = \frac{1}{\sqrt{2}} \left( e^{i\omega T} |z+\rangle + e^{-i\omega T} |z-\rangle \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega T} \\ e^{-i\omega T} \end{pmatrix}$$

$$= a |y+\rangle + b |y-\rangle = \frac{a}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} + \frac{b}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

or

$$a + b = e^{i\omega T} \quad i(a - b) = e^{-i\omega T}$$

or

$$\begin{cases} 2a = e^{i\omega T} - ie^{-i\omega T} \\ 2b = e^{i\omega T} + ie^{-i\omega T} \end{cases}$$

so that

$$|\psi(t)\rangle = e^{-i\hat{H}(t-T)/\hbar} (a |y+\rangle + b |y-\rangle) = ae^{i\omega (t-T)} |y+\rangle + be^{-i\omega (t-T)} |y-\rangle$$

and

$$|\psi(2T)\rangle = \frac{1}{2\sqrt{2}} \left( (e^{i\omega T} - ie^{-i\omega T})e^{i\omega T} \begin{pmatrix} 1 \\ i \end{pmatrix} + (e^{i\omega T} + ie^{-i\omega T})e^{-i\omega T} \begin{pmatrix} 1 \\ -i \end{pmatrix} \right)$$

Finally,

$$\langle S_x = + | \psi(2T) \rangle$$

$$= \frac{1}{\sqrt{2}} (1, 1) \frac{1}{2\sqrt{2}} \left( (e^{i\omega T} - ie^{-i\omega T})e^{i\omega T} \begin{pmatrix} 1 \\ i \end{pmatrix} + (e^{i\omega T} + ie^{-i\omega T})e^{-i\omega T} \begin{pmatrix} 1 \\ -i \end{pmatrix} \right)$$

$$= \frac{1}{2} \left( (1-i) + (1+i) \cos 2\omega T \right)$$

and

$$Prob = \frac{1}{4} \left( (1 + \cos 2\omega T)^2 + (1 - \cos 2\omega T)^2 \right)$$

$$= \frac{1}{4} (2 + 2 \cos^2 2\omega T) = \frac{1}{2} (1 + \cos^2 2\omega T)$$

as in part (1).

(3) Using the density operator formalism.

The initial system density operator is

$$\hat{\rho} = |\psi(0)\rangle \langle \psi(0)| = |x+\rangle \langle x+|$$

$$= \frac{1}{2} \left( |z+\rangle \langle z+| + |z+\rangle \langle z-| + |z-\rangle \langle z+| + |z-\rangle \langle z-| \right) = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

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During the time interval $0 \leq t < T$ we have
\[
\hat{H} = -\hbar \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]
The equation of motion for the density operator is
\[
\frac{d\hat{\rho}(t)}{dt} = -\frac{i}{\hbar} \left[ \hat{H}(t), \hat{\rho}(t) \right]
\]
and the probability of measuring $|S_x = +\rangle = |x+\rangle$ at time $t$ is
\[
P(t) = Tr(\hat{\rho}(t) |x+\rangle \langle x+|)
\]
Now assuming that
\[
\hat{\rho}(t) = \begin{pmatrix} a & b \\ c & d \end{pmatrix}
\]
we have
\[
\begin{pmatrix} \dot{a} \\ \dot{b} \\ \dot{c} \\ \dot{d} \end{pmatrix} = i\omega \left[ \hat{\sigma}_z, \hat{\rho}(t) \right]
\]
\[
= i\omega \left( \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} - \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right)
\]
\[
= i\omega \begin{pmatrix} 0 & 2b \\ -2c & 0 \end{pmatrix}
\]
so that
\[
\dot{a} = 0 \rightarrow a(t) = a(0) = \frac{1}{2}
\]
\[
\dot{d} = 0 \rightarrow d(t) = d(0) = \frac{1}{2}
\]
\[
\dot{b} = 2i\omega b \rightarrow b(t) = \frac{1}{2} e^{2i\omega t}
\]
\[
\dot{c} = -2i\omega c \rightarrow c(t) = \frac{1}{2} e^{-2i\omega t}
\]
so that
\[
\hat{\rho}(t) = \frac{1}{2} \begin{pmatrix} 1 & e^{2i\omega t} \\ e^{-2i\omega t} & 1 \end{pmatrix}
\]
or
\[
\hat{\rho}(T) = \frac{1}{2} \begin{pmatrix} 1 & e^{2i\omega T} \\ e^{-2i\omega T} & 1 \end{pmatrix}
\]
Now during the time interval $T \leq t \leq 2T$ we have
\[
\hat{H} = -\hbar \omega \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}
\]
The initial density operator is now $\hat{\rho}(T)$. The equations of motion are
\[
\begin{pmatrix} \dot{a} \\ \dot{b} \\ \dot{c} \\ \dot{d} \end{pmatrix} = i\omega \left[ \hat{\sigma}_y, \hat{\rho}(t) \right]
\]
\[
= i\omega \left( \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} - \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right)
\]
\[
= -\omega \begin{pmatrix} -(b + c) & (a - d) \\ (a - d) & (b + c) \end{pmatrix}
\]
so that

\[ \dot{a} = \omega(b + c) \quad a(T) = \frac{1}{2} \quad \dot{b} = -\omega(a - d) \quad b(T) = \frac{1}{2} e^{2i\omega T} \]
\[ \dot{c} = -\omega(a - d) \quad c(T) = \frac{1}{2} e^{-2i\omega T} \quad \dot{d} = -\omega(b + c) \quad d(T) = \frac{1}{2} \]

These equations say that

\[ \dot{a} = -\dot{d} \rightarrow a = -d + G_1 \]
\[ \dot{b} = \dot{c} \rightarrow b = c + G_2 \]

The boundary conditions then give

\[ a(T) = -d(T) + G_1 = a(T) + d(T) = 1 \]
\[ b(T) = c(T) + G_2 = b(T) - c(T) = \frac{1}{2} e^{2i\omega T} - \frac{1}{2} e^{-2i\omega T} = i \sin 2\omega T \]

so that

\[ a(t) = -d(t) + 1 \]
\[ b(t) = c(t) + i \sin 2\omega T \]

Therefore, we have the equations

\[ \dot{a} = \omega(2b - i \sin 2\omega T) \quad a(T) = \frac{1}{2} \quad \dot{b} = -\omega(2a - 1) \quad b(T) = \frac{1}{2} e^{2i\omega T} \]

Therefore, we have

\[ \ddot{a} = 2\omega \dot{b} = -4\omega^2 a + 2\omega^2 \]
\[ \ddot{b} = -2\omega \dot{a} = -4\omega^2 b + 2i\omega^2 \sin 2\omega T \]

which have solutions

\[ a(t) = \text{Re} e^{2i\omega t} + \text{Se}^{-2i\omega t} + \frac{1}{2} \]
\[ b(t) = U e^{2i\omega t} + V e^{-2i\omega t} + \frac{1}{2} \sin 2\omega T \]

In order for the equations to be consistent we must have

\[ \dot{a} = \omega(2b - i \sin 2\omega T) \]
\[ 2i\omega \left( \text{Re} e^{2i\omega t} - \text{Se}^{-2i\omega t} \right) = 2\omega \left( U e^{2i\omega t} + V e^{-2i\omega t} + \frac{i}{2} \sin 2\omega T \right) - i \sin 2\omega T \]
\[ i \left( \text{Re} e^{2i\omega t} - \text{Se}^{-2i\omega t} \right) = \left( U e^{2i\omega t} + V e^{-2i\omega t} \right) \]

or

\[ iR = U \quad \text{and} \quad -iS = V \]

Similarly, we must have

\[ \dot{b} = -\omega(2a - 1) \]
\[ 2i\omega \left( U e^{2i\omega t} - V e^{-2i\omega t} \right) = -2\omega \left( \text{Re} e^{2i\omega t} + \text{Se}^{-2i\omega t} \right) \]
\[ (U e^{2i\omega t} - V e^{-2i\omega t}) = i \left( \text{Re} e^{2i\omega t} + \text{Se}^{-2i\omega t} \right) \]

or

\[ iR = U \quad \text{and} \quad -iS = V \]

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which is identical to the above result.

So we have

\[ a(t) = \Re 2i\omega t + S e^{-2i\omega t} + \frac{1}{2} \]
\[ b(t) = i\Re 2i\omega t - iS e^{-2i\omega t} + \frac{i}{2} \sin 2\omega T \]

Now the boundary conditions are

\[ a(T) = \frac{1}{2} = \Re 2i\omega T + S e^{-2i\omega T} + \frac{1}{2} \]
\[ \Re 2i\omega T + S e^{-2i\omega T} = 0 \]
\[ b(T) = \frac{1}{2} e^{2i\omega T} = i\Re 2i\omega T - iS e^{-2i\omega T} + \frac{i}{2} \sin 2\omega T \]
\[ \Re 2i\omega T - S e^{-2i\omega T} = \frac{1}{2i} \left( e^{2i\omega T} - i \sin 2\omega T \right) \]
\[ = \frac{1}{2i} \left( e^{2i\omega T} - \frac{1}{2} e^{2i\omega T} + \frac{1}{2} e^{-2i\omega T} \right) = \frac{1}{i} \cos 2\omega T \]

(9.1)

or

\[ 2\Re 2i\omega T = \frac{1}{2} \cos 2\omega T \to R = \frac{1}{2\pi} e^{-2i\omega T} \cos 2\omega T \]
\[ 2S e^{-2i\omega T} = -\frac{1}{4} \cos 2\omega T \to S = -\frac{1}{2\pi} e^{2i\omega T} \cos 2\omega T \]

Therefore,

\[ a(t) = \Re 2i\omega t + S e^{-2i\omega t} + \frac{1}{2} = \frac{1}{2i} \cos 2\omega T \left( e^{-2i\omega T} e^{2i\omega t} - e^{2i\omega T} S e^{-2i\omega t} \right) + \frac{1}{2} \]

\[ b(t) = i\Re 2i\omega t - iS e^{-2i\omega t} + \frac{i}{2} \sin 2\omega T \]
\[ = \frac{1}{2} \cos 2\omega T \left( e^{-2i\omega T} e^{2i\omega t} + e^{2i\omega T} S e^{-2i\omega t} \right) + \frac{i}{2} \sin 2\omega T \]
\[ c(t) = b(t) - i \sin 2\omega T = \frac{1}{2} \cos 2\omega T \left( e^{-2i\omega T} e^{2i\omega t} + e^{2i\omega T} S e^{-2i\omega t} \right) - \frac{i}{2} \sin 2\omega T \]
\[ d(t) = 1 - a(t) = \frac{1}{2} - \frac{1}{2\pi} \cos 2\omega T \left( e^{-2i\omega T} e^{2i\omega t} - e^{2i\omega T} S e^{-2i\omega t} \right) \]

Consistency checks:

\[ \text{Tr} \hat{\rho} = a + d = 1 \text{ (true) and } \hat{\rho} = \hat{\rho}^+ \to b^* = c \text{ (true)} \]

Thus,

\[ \hat{\rho}(t) = \begin{pmatrix}
\frac{1}{2} \cos 2\omega T \left( e^{2i\omega (t-T)} - e^{-2i\omega (t-T)} \right) + \frac{1}{2} \\
\frac{1}{2} \cos 2\omega T \left( e^{2i\omega (t+T)} + e^{-2i\omega (t-T)} \right) + \frac{1}{2} \sin 2\omega T \\
\frac{1}{2} \cos 2\omega T \left( e^{2i\omega (t-T)} + e^{-2i\omega (t+T)} \right) - \frac{1}{2} \sin 2\omega T \\
\frac{1}{2} \cos 2\omega T \left( e^{2i\omega (t+T)} - e^{-2i\omega (t-T)} \right) + \frac{1}{2} \sin 2\omega T \\
\end{pmatrix} \]

Now

\[ P(2T) = \text{Tr}(\hat{\rho}(2T) \mid x+ \rangle \langle x+ \mid) \]
\[ = \frac{1}{2} \text{Tr} \left( \begin{pmatrix}
\cos 2\omega T \sin 2\omega T + \frac{1}{2} & \cos^2 2\omega T + \frac{i}{2} \sin 2\omega T & \frac{1}{2} \cos 2\omega T \left( e^{2i\omega (t-T)} + e^{-2i\omega (t-T)} \right) + \frac{i}{2} \sin 2\omega T \\
\cos^2 2\omega T - \frac{1}{2} \sin 2\omega T & \frac{1}{2} - \cos 2\omega T \sin 2\omega T & \frac{1}{2} \cos 2\omega T \left( e^{2i\omega (t-T)} - e^{-2i\omega (t-T)} \right) + \frac{1}{2} \sin 2\omega T \\
\cos^2 2\omega T - \frac{1}{2} \sin 2\omega T + \frac{1}{2} \cos 2\omega T & \frac{1}{2} - \cos 2\omega T \sin 2\omega T & \frac{1}{2} - \frac{1}{2\pi} \cos 2\omega T \left( e^{2i\omega (t-T)} + e^{-2i\omega (t-T)} \right) + \frac{i}{2} \sin 2\omega T \\
\end{pmatrix} \right) \]
\[ = \frac{1}{2} \left( 1 + 2 \cos^2 2\omega T \right) \]
which agrees with earlier results.

9.7.19 What happens in the Stern-Gerlach box?

An atom with spin $= \frac{1}{2}$ 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?

We have

$$\hat{H} = -\vec{\mu} \cdot \vec{B} = \frac{|e|}{2mc} \hat{\sigma}_x = \hbar \omega \hat{\sigma}_x$$

The Schrodinger equation is

$$i\hbar \frac{d}{dt} \begin{pmatrix} a \\ b \end{pmatrix} = \hbar \omega \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \hbar \omega \begin{pmatrix} b \\ a \end{pmatrix} \rightarrow i\dot{a} = \omega b \quad , \quad i\dot{b} = \omega a$$

This gives

$$\dot{a} + \omega^2 a = 0 \rightarrow a(t) = \alpha e^{i\omega t} + \beta e^{-i\omega t}$$

$$b(t) = \frac{1}{i\omega} \dot{a} = -\alpha e^{i\omega t} + \beta e^{-i\omega t}$$

Now,

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

Therefore,

$$\alpha + \beta = 1 \rightarrow \alpha = \beta = \frac{1}{2}$$

and

$$|\psi(t)\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} e^{i\omega t} + e^{-i\omega t} \\ -e^{i\omega t} + e^{-i\omega t} \end{pmatrix} = \begin{pmatrix} \cos \omega t \\ -i \sin \omega t \end{pmatrix} = \cos \omega t \begin{pmatrix} 1 \\ 0 \end{pmatrix} - i \sin \omega t \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Now,

$$P(-z; t) = |\langle -z | \psi(t) \rangle|^2 = \sin^2 \omega t = \frac{1 - \cos 2\omega t}{2}$$

Thus, the probability = 1 if

$$1 - \cos 2\omega t = 2 \rightarrow \cos 2\omega t = -1 \rightarrow t = \frac{2n + 1}{2\omega} \pi = (2n + 1) \frac{mc\pi}{|e| B}$$

Alternatively, we have

$$\hat{U} = e^{-i\hat{H}t/\hbar} = e^{-i\omega t \hat{\sigma}_x} = \cos \omega t \hat{I} - i\hat{\sigma}_x \sin \omega t$$

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Then
\[
|\psi(t)\rangle = \hat{U} |\psi(0)\rangle = \left(\cos \omega t \hat{I} - i \hat{\sigma}_y \sin \omega t\right) |+\rangle = \frac{1}{\sqrt{2}} \left(\cos \omega t \hat{I} - i \hat{\sigma}_x \sin \omega t\right) (|+\rangle + |-\rangle)
\]
\[
= \frac{1}{\sqrt{2}} \left((\cos \omega t - i \sin \omega t) |+\rangle + (\cos \omega t + i \sin \omega t) |-\rangle\right)
\]
\[
= \frac{1}{\sqrt{2}} \left(e^{-i\omega t} |+\rangle + e^{i\omega t} |-\rangle\right)
\]
\[
= \cos \omega t |+\rangle - i \sin \omega t |-\rangle
\]
as above.

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 \( t \).

We have \( \vec{B} = B_0 \hat{e}_x, \hat{H} = \omega_0 \hat{S}_x \) and

\[
|\psi(0)\rangle = |1, 1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
\]

From problem 9.7.15 we have

\[
|1, 1\rangle_x = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2} |1, 1\rangle + \frac{\sqrt{2}}{2} |1, 0\rangle + \frac{1}{2} |1, -1\rangle
\]
\[
|1, 0\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} |1, 1\rangle - \frac{1}{\sqrt{2}} |1, -1\rangle
\]
\[
|1, -1\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2} |1, 1\rangle - \frac{\sqrt{2}}{2} |1, 0\rangle + \frac{1}{2} |1, -1\rangle
\]

Therefore,

\[
x \langle 1, 1 | \psi(0) \rangle = x \langle 1, 1 | 1, 1 \rangle = \frac{1}{2}
\]
\[
x \langle 1, 0 | \psi(0) \rangle = x \langle 1, 0 | 1, 1 \rangle = \frac{1}{\sqrt{2}}
\]
\[
x \langle 1, -1 | \psi(0) \rangle = x \langle 1, -1 | 1, 1 \rangle = \frac{1}{2}
\]

Now,

\[
\hat{H} |1, 1\rangle_x = \omega_0 \hat{S}_x |1, 1\rangle_x = \hbar \omega_0 |1, 1\rangle_x
\]
\[
\hat{H} |1, 0\rangle_x = \omega_0 \hat{S}_x |1, 0\rangle_x = 0
\]
\[
\hat{H} |1, -1\rangle_x = \omega_0 \hat{S}_x |1, -1\rangle_x = -\hbar \omega_0 |1, -1\rangle_x
\]

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Then,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = e^{-i\hat{H}t/\hbar} \left( \frac{1}{2} |1,1\rangle_x + \frac{1}{\sqrt{2}} |1,0\rangle_x + \frac{1}{2} |1,-1\rangle_x \right)$$

$$= \frac{1}{2} e^{-i\omega_0 t} |1,1\rangle_x + \frac{1}{\sqrt{2}} |1,0\rangle_x + \frac{1}{2} e^{i\omega_0 t} |1,-1\rangle_x$$

Going back to the $z$-basis we have

$$|\psi(t)\rangle = \frac{1}{2} e^{-i\omega_0 t} \frac{1}{2} \begin{pmatrix} 1 & \sqrt{2} \\ 1 & 1 \end{pmatrix} + \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \frac{1}{2} e^{i\omega_0 t} \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{2} \\ -\sqrt{2} & 1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 + \cos \omega_0 t \\ -\sqrt{2} \sin \omega_0 t \\ -1 + \cos \omega_0 t \end{pmatrix}$$

Finally,

$$P(S_z = -\hbar; t) = |\langle 1, -1 | \psi(t) \rangle|^2 = |\langle 0, 0, 1, 1 | \psi(t) \rangle|^2$$

$$= \left| \frac{1}{2} (-1 + \cos \omega_0 t) \right|^2 = \sin^2 \left( \frac{\omega_0 t}{2} \right)$$

NOTE: When $\omega_0 t = \pi$, $P(S_z = -\hbar; t = \pi/\omega_0) = 1$. Since $\hat{U}(t) = e^{-i\hat{H}t/\hbar} = e^{-i\omega_0 t \hat{S}_z/\hbar}$, when $\omega_0 t = \pi$, the spin has precessed by 180° about the $x$-axis, turning a spin-up along the $z$-direction state into a spin-down along the $z$-direction state.

### 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.

We have $\vec{B} = B_0 \hat{z} + B_1 \hat{x}$ so that the $\vec{B}$-axis (call it $z'$) makes and angle

$$\theta = \tan^{-1} \frac{B_1}{B_0}$$

with the $z$-axis. Therefore

$$|+z'\rangle = \cos \frac{\theta}{2} |+z\rangle + \sin \frac{\theta}{2} |-z\rangle$$

$$|-z'\rangle = -\sin \frac{\theta}{2} |+z\rangle + \cos \frac{\theta}{2} |-z\rangle$$

$$|\psi(0)\rangle = |+z\rangle$$
(a) At $t = 0^+$, what are the amplitudes for finding the system with spin projections $m' = 1/2$ with respect to the $z'$-axis?

We then have
\[
\begin{align*}
P(+z'; t = 0^+) &= |\langle +z' | \psi(0) \rangle|^2 |\langle +z' | +z \rangle|^2 = \cos^2 \frac{\theta}{2} \\
P(-z'; t = 0^+) &= |\langle -z' | \psi(0) \rangle|^2 |\langle -z' | +z \rangle|^2 = \sin^2 \frac{\theta}{2}
\end{align*}
\]

(b) What is the time development of the energy eigenstates with respect to the $z'$ direction, during the time interval $0 < t < T$?

In this interval, the Hamiltonian is
\[
\hat{H} = -\mu \cdot \vec{B} = -\mu_0 (B_0 \sigma_z + B_1 \sigma_x) = -\mu_0 \left( \begin{array}{cc} B_0 & B_1 \\ B_1 & -B_0 \end{array} \right) = -\mu_0 B \left( \begin{array}{cc} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{array} \right)
\]

where $B = \sqrt{B_0^2 + B_1^2}$. The corresponding eigenvalues/eigenvectors are
\[
\begin{align*}
E_\pm &= \mp \mu_0 B = \mp \mu_0 \sqrt{B_0^2 + B_1^2} \\
|E_\pm \rangle &= |\mp z' \rangle
\end{align*}
\]
as expected!

(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 $\theta$ between the $z$ and $z'$ axes and the frequency $\omega_0 = \mu_0 B_0 / \hbar$]

Using spectral decomposition, we then have
\[
\hat{U}(t) = e^{-i\hat{H}t/\hbar} = e^{-i\mu_0 Bt/\hbar} | -z' \rangle \langle -z' | + e^{i\mu_0 Bt/\hbar} | +z' \rangle \langle +z' |
\]

so that
\[
|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = \hat{U}(t) |+z\rangle = e^{-i\mu_0 Bt/\hbar} | -z' \rangle \langle -z' | +z + e^{i\mu_0 Bt/\hbar} | +z' \rangle \langle +z' | +z = -\sin \frac{\theta}{2} e^{-i\mu_0 Bt/\hbar} | -z' \rangle + \cos \frac{\theta}{2} e^{i\mu_0 Bt/\hbar} | +z'
\]

and
\[
P(-z; T) = |\langle -z | \psi(T) \rangle|^2 = \left| -\sin \frac{\theta}{2} e^{-i\mu_0 Bt/\hbar} (-z | -z') + \cos \frac{\theta}{2} e^{i\mu_0 Bt/\hbar} (-z | +z') \right|^2
\]

\[
= \left| -\sin \frac{\theta}{2} \cos \frac{\theta}{2} e^{-i\mu_0 Bt/\hbar} + \sin \frac{\theta}{2} \cos \frac{\theta}{2} e^{i\mu_0 Bt/\hbar} \right|^2 = 4 \sin^2 \frac{\theta}{2} \cos^2 \frac{\theta}{2} \sin^2 \frac{\mu_0 Bt}{\hbar}
\]

9.7.22 Neutron interferometer

In a classic table-top experiment (neutron interferometer), a monochromatic neutron beam ($\lambda = 1.445\text{Å}$) 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:
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.

This is a spinor state interference problem. We consider a neutron in the beam. In the region where the magnetic field is $\vec{B}$ the Schrodinger equation for the uncharged neutron is

\[
\left( -\frac{\hbar^2}{2m} \nabla^2 - \mu \vec{\sigma} \cdot \vec{B} \right) \psi = E \psi
\]

(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.

Suppose that $\vec{B}$ is uniform and constant. Then

\[
\psi(t_1) = e^{-i\vec{H}(t_1-t_0)/\hbar} \psi(t_0)
\]

where

\[
t_0 = \text{time when neutron enters field region}
\]

\[
t_1 = \text{time when neutron leaves field region}
\]

We then write

\[
\psi(t) = \psi(\vec{r},t)\psi(\vec{s},t) = \text{(space - part)(spin - part)}
\]

which implies that

\[
\psi(\vec{r},t_1) = e^{i\left(\frac{\hbar^2}{2m} \nabla^2\right)(t_1-t_0)/\hbar} \psi(\vec{r},t_0)
\]

\[
\psi(\vec{s},t_1) = e^{i(\mu \vec{\sigma} \cdot \vec{B})(t_1-t_0)/\hbar} \psi(\vec{s},t_0)
\]

The interference effects arise from the action of $\vec{B}$ on the spin-part of the wave function.
Now $\psi(\vec{r}, t)$ is the wave function of a free particle so that

$$t_1 - t_0 = \frac{L}{v} = \frac{mL}{\hbar k}$$

and thus

$$\psi(\vec{s}, t_1) = e^{i(\mu \vec{\sigma} \cdot \vec{B})mL\lambda/2\pi\hbar^2} \psi(\vec{s}, t_0)$$

where

$$k = \frac{2\pi}{\lambda} = \frac{mv}{\hbar} = \text{neutron wave number}$$

The intensity of the two beams at $D$ is proportional to

$$|\psi_D^{(1)}(\vec{r}, t)\psi_D^{(1)}(\vec{s}, t) + \psi_D^{(2)}(\vec{r}, t)\psi_D^{(2)}(\vec{s}, t)|^2 \propto |\psi_D^{(1)}(\vec{s}, t) + \psi_D^{(2)}(\vec{s}, t)|^2$$

$$= |\psi(\vec{s}, t_0) + \psi(\vec{s}, t_0)e^{i(\mu \vec{\sigma} \cdot \vec{B})mL\lambda/2\pi\hbar^2}|^2 = |\psi(\vec{s}, t_0)|^2 \left(1 + e^{i(\mu \vec{\sigma} \cdot \vec{B}/B)mL\lambda B/2\pi\hbar^2}\right)^2$$

Now,

$$\vec{\sigma} \cdot \vec{B} = \pm \sigma$$

depending if $\vec{\sigma}$ is parallel or antiparallel to $\vec{B}$. We then have

$$I = \text{intensity of interference at } D$$

$$= \left|1 + \cos \frac{\mu m\lambda B}{2\pi\hbar^2} + i\sigma \cdot \frac{\vec{B}}{B} \sin \frac{\mu m\lambda B}{2\pi\hbar^2}\right|^2$$

$$= \left(1 + \cos \frac{\mu m\lambda B}{2\pi\hbar^2}\right)^2 + \sin^2 \frac{\mu m\lambda B}{2\pi\hbar^2}$$

$$= 4 \cos^2 \frac{\mu m\lambda B}{4\pi\hbar^2}$$

(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.

The separation between the maxima is given by

$$\frac{\mu m\lambda \Delta B}{4\pi\hbar^2} = \pi \rightarrow \Delta B = \frac{4\pi^2 \hbar^2}{\mu m\lambda} = \frac{4\pi^2 \hbar^2}{\mu \lambda} = \frac{8\pi^2 \hbar c}{g_n e \lambda}$$
9.7.23 Magnetic Resonance

A particle of spin 1/2 and magnetic moment \( \mu \) 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 \( t > 0 \).

We have a spin = 1/2 particle in a magnetic field

\[ \vec{B} = B_0 \hat{z} + B_1 \hat{x} \cos \omega t - B_1 \hat{y} \sin \omega t \]

The Hamiltonian is

\[ \hat{H} = -\gamma \hat{S} \cdot \vec{B} = -\frac{\hbar}{2} (B_0 \hat{\sigma}_z + B_1 \cos \omega t \hat{\sigma}_x - B_1 \sin \omega t \hat{\sigma}_y) \]

We first make a transformation to a rotating frame of reference. The equations

\[ i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \\
|\psi_r(t)\rangle = e^{-i\omega t \hat{S}_z / \hbar} |\psi(t)\rangle \]

give

\[ \hbar \frac{d}{dt} e^{i\omega t \hat{S}_z / \hbar} |\psi(t)\rangle = \hat{H} e^{i\omega t \hat{S}_z / \hbar} |\psi(t)\rangle \]
\[ i\hbar \frac{d}{dt} |\psi_r(t)\rangle = \omega e^{-i\omega t \hat{S}_z / \hbar} \hat{S}_z e^{i\omega t \hat{S}_z / \hbar} |\psi_r(t)\rangle + e^{-i\omega t \hat{S}_z / \hbar} \hat{H} e^{i\omega t \hat{S}_z / \hbar} |\psi_r(t)\rangle \]
\[ i\hbar \frac{d}{dt} |\psi_r(t)\rangle = \frac{\hbar}{2} \hat{\sigma}_z |\psi_r(t)\rangle \]
\[ -\gamma \frac{\hbar}{2} e^{-i\omega t \hat{S}_z / \hbar} (B_0 \hat{\sigma}_z + B_1 \cos \omega t \hat{\sigma}_x - B_1 \sin \omega t \hat{\sigma}_y) e^{i\omega t \hat{S}_z / \hbar} |\psi_r(t)\rangle \]
\[ i\hbar \frac{d}{dt} |\psi_r(t)\rangle = \frac{\hbar}{2} \hat{\sigma}_z |\psi_r(t)\rangle \]
\[ -\gamma \frac{\hbar}{2} \left( B_0 e^{-i\omega t \hat{S}_z / 2} \hat{\sigma}_z e^{i\omega t \hat{S}_z / 2} + B_1 \cos \omega t e^{-i\omega t \hat{S}_z / 2} \hat{\sigma}_x e^{i\omega t \hat{S}_z / 2} - B_1 \sin \omega t e^{-i\omega t \hat{S}_z / 2} \hat{\sigma}_y e^{i\omega t \hat{S}_z / 2} \right) |\psi_r(t)\rangle \]
\[ i\hbar \frac{d}{dt} |\psi_r(t)\rangle = \frac{\hbar}{2} \hat{\sigma}_z |\psi_r(t)\rangle \]
\[ -\gamma \frac{\hbar}{2} \left( B_0 \hat{\sigma}_z + B_1 \cos \omega t e^{-i\omega t \hat{S}_z / 2} \hat{\sigma}_x e^{i\omega t \hat{S}_z / 2} - B_1 \sin \omega t e^{-i\omega t \hat{S}_z / 2} \hat{\sigma}_y e^{i\omega t \hat{S}_z / 2} \right) |\psi_r(t)\rangle \]

Now

\[ e^{\pm i\omega t \hat{S}_z / 2} = \cos \frac{\omega t}{2} \pm i \hat{\sigma}_z \sin \frac{\omega t}{2} \]

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and therefore,

\[ e^{-i\omega \hat{\sigma}_z/2} \hat{\sigma}_x e^{i\omega \hat{\sigma}_z/2} = \left( \cos \frac{\omega t}{2} - i \hat{\sigma}_z \sin \frac{\omega t}{2} \right) \hat{\sigma}_x \left( \cos \frac{\omega t}{2} + i \hat{\sigma}_z \sin \frac{\omega t}{2} \right) \]

\[ = \cos^2 \frac{\omega t}{2} \hat{\sigma}_x + i \cos \frac{\omega t}{2} \sin \frac{\omega t}{2} [\hat{\sigma}_x, \hat{\sigma}_z] + \sin^2 \frac{\omega t}{2} \hat{\sigma}_x \hat{\sigma}_z \]

\[ = \cos^2 \frac{\omega t}{2} \hat{\sigma}_x + i \cos \frac{\omega t}{2} \sin \frac{\omega t}{2} (-2i \hat{\sigma}_y) + \sin^2 \frac{\omega t}{2} (i \hat{\sigma}_y \hat{\sigma}_z) \]

\[ = \cos^2 \frac{\omega t}{2} \hat{\sigma}_x + 2 \cos \frac{\omega t}{2} \sin \frac{\omega t}{2} \hat{\sigma}_y - \sin^2 \frac{\omega t}{2} \hat{\sigma}_x \]

\[ = \cos \omega t \hat{\sigma}_x + \sin \omega t \hat{\sigma}_y \]

and similarly,

\[ e^{-i\omega \hat{\sigma}_y/2} \hat{\sigma}_y e^{i\omega \hat{\sigma}_y/2} = -\sin \omega t \hat{\sigma}_x + \cos \omega t \hat{\sigma}_y \]

Therefore,

\[ i\hbar \frac{d}{dt} |\psi_r(t)\rangle = \frac{\hbar \omega}{2} \hat{\sigma}_z |\psi_r(t)\rangle \]

\[ - \gamma \frac{\hbar}{2} \left( B_0 \hat{\sigma}_x + B_1 \cos \omega t (\cos \omega t \hat{\sigma}_x + \sin \omega t \hat{\sigma}_y) \right) |\psi_r(t)\rangle \]

\[ i\hbar \frac{d}{dt} |\psi_r(t)\rangle = \frac{\hbar \omega}{2} \hat{\sigma}_x |\psi_r(t)\rangle \]

\[ - \gamma \frac{\hbar}{2} \left( B_0 \hat{\sigma}_y + B_1 \left( \frac{\hat{\sigma}_x}{2} + \frac{\cos 2\omega t}{2} \hat{\sigma}_x + \frac{1}{2} \sin 2\omega t \hat{\sigma}_y \right) \right) |\psi_r(t)\rangle \]

\[ i\hbar \frac{d}{dt} |\psi_r(t)\rangle = \frac{\hbar(\omega - \omega_0)}{2} \hat{\sigma}_z |\psi_r(t)\rangle - \frac{\hbar \omega_1}{2} \hat{\sigma}_x |\psi_r(t)\rangle = \frac{\hbar}{2} \left( (\omega - \omega_0) \hat{\sigma}_z - \omega_1 \hat{\sigma}_x \right) |\psi_r(t)\rangle \]

where \( \omega_0 = \gamma B_0 \) and \( \omega_1 = \gamma B_1 \)

We then have

\[ i\hbar \frac{d}{dt} |\psi_r(t)\rangle = \frac{\hbar}{2} \left( (\omega - \omega_0) \hat{\sigma}_z - \omega_1 \hat{\sigma}_x \right) |\psi_r(t)\rangle \]

Manipulating this equation we get

\[ \frac{d}{dt} |\psi_r(t)\rangle = -\frac{\Omega}{2} \hat{\sigma} |\psi_r(t)\rangle \]

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where
\[ \sigma = \frac{\omega_0 - \omega}{\Omega} \sigma_z - \frac{\omega_1}{\Omega} \sigma_x \] and \[ \Omega^2 = (\omega - \omega_0)^2 + \omega_1^2 \]

Since \( \sigma^2 = I \) we can write
\[ |\psi_r(t)\rangle = e^{-i\frac{\Omega t}{2} \sigma} |\psi_r(0)\rangle \]
and then
\[ e^{-i\omega t \hat{S}_z / \hbar} |\psi(t)\rangle = e^{-i\frac{\Omega t}{2} \sigma} |\psi(0)\rangle \]
\[ |\psi(t)\rangle = e^{i\omega t \hat{S}_z / \hbar} e^{-i\frac{\Omega t}{2} \sigma} |\psi(0)\rangle \]

The last equation is the time development equation for the system state vector. The initial state is
\[ |\psi(0)\rangle = |z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]

Therefore,
\[ |\psi(t)\rangle = e^{i\omega t \hat{S}_z / \hbar} \left( \cos \frac{\Omega t}{2} - i \sin \frac{\Omega t}{2} \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]
\[ = e^{i\omega t \hat{S}_z / \hbar} \left( \cos \frac{\Omega t}{2} - i \sin \frac{\Omega t}{2} \left( \frac{\omega - \omega_0}{\Omega} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{\omega_1}{\Omega} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right) \right) \]
\[ = e^{i\omega t \hat{S}_z / \hbar} \left( \cos \frac{\Omega t}{2} - i \frac{\omega - \omega_0}{\Omega} \sin \frac{\Omega t}{2} \right) \left( \cos \frac{\Omega t}{2} - i \frac{\omega - \omega_0}{\Omega} \sin \frac{\Omega t}{2} e^{i\omega t/2} \right) \]

Therefore, finally
\[ |\psi(t)\rangle = \left( \cos \frac{\Omega t}{2} - i \frac{\omega - \omega_0}{\Omega} \sin \frac{\Omega t}{2} e^{i\omega t/2} \right) \]
\[ = \left( \cos \frac{\Omega t}{2} - i \frac{\omega - \omega_0}{\Omega} \sin \frac{\Omega t}{2} e^{i\omega t/2} \right) |z\rangle + i \frac{\omega_1}{\Omega} \sin \frac{\Omega t}{2} e^{-i\omega t/2} |z\rangle \]

and
\[ P(z-) = |\langle z- | \psi(t) \rangle|^2 = \left| \frac{\omega_1}{\Omega} \sin \frac{\Omega t}{2} e^{-i\omega t/2} \right|^2 = \left( \frac{\omega_1}{\Omega} \right)^2 \sin^2 \frac{\Omega t}{2} \]

Alternative solution using differential equations

We have
\[ \hat{H} = -\gamma \vec{S} \cdot \vec{B} = -\frac{\hbar}{2} \left( \omega_0 \sigma_z + \omega_1 \cos \omega t \sigma_x - \omega_1 \sin \omega t \sigma_y \right) \]
\[ = -\frac{\hbar}{2} \omega_0 \sigma_z - \frac{\hbar}{2} \omega_1 \left( \begin{array}{cc} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{array} \right) \]

Then
\[ i \hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \]
\[ i \left( \begin{array}{c} a \\ b \end{array} \right) = -\frac{1}{2} \omega_0 \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) \left( \begin{array}{c} a \\ b \end{array} \right) - \frac{1}{2} \omega_1 \left( \begin{array}{cc} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{array} \right) \left( \begin{array}{c} a \\ b \end{array} \right) \]

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so that 
\[
\dot{a} = \frac{i}{2} \omega_0 a + \frac{i}{2} \omega_1 e^{i\omega t} b \\
\dot{b} = -\frac{i}{2} \omega_0 b + \frac{i}{2} \omega_1 e^{-i\omega t} a
\]

We guess solutions of the form 
\[
a = \alpha e^{i\omega_0 t/2}, \quad b = \beta e^{-i\omega_0 t/2}
\]

which gives 
\[
\dot{\alpha} = i \frac{\omega_1}{2} e^{i(-\omega_0 + \omega)t} \beta \\
\dot{\beta} = i \frac{\omega_1}{2} e^{-i(-\omega_0 + \omega)t} \alpha
\]

Now assume that 
\[
\alpha = A_1 e^{i(-\omega_0 + \omega + \Omega)t} \\
\beta = A_2 e^{i\Omega t}
\]

Substitution gives 
\[
\begin{aligned}
(-\omega_0 + \omega + \Omega) A_1 - \frac{\omega_1}{2} A_2 &= 0 \\
-\frac{\omega_1}{2} A_1 + \Omega A_2 &= 0
\end{aligned}
\]

These homogeneous equations have a non-trivial solution only if 
\[
\begin{vmatrix}
-\omega_0 + \omega + \Omega & -\frac{\omega_1}{2} \\
-\frac{\omega_1}{2} & \Omega
\end{vmatrix} = 0 \\
= \Omega (-\omega_0 + \omega + \Omega) - \frac{\omega_1^2}{4} = 0
\]

so that 
\[
\Omega = \frac{\omega - \omega_0}{2} \pm \frac{1}{2} \sqrt{(\omega - \omega_0)^2 + \omega_1^2} = \frac{\omega - \omega_0}{2} \pm \frac{\Omega}{2}
\]

where 
\[
\Omega = \sqrt{(\omega - \omega_0)^2 + \omega_1^2}
\]

Therefore, the most general solutions are 
\[
\beta = A_{2+} e^{i\Omega t} + A_{2-} e^{-i\Omega t} \\
\alpha = -\frac{\omega_1}{\omega_1} e^{i(-\omega_0 + \omega)t} \beta = \frac{2}{\omega_1} e^{i(-\omega_0 + \omega)t} \left( \Omega+ A_{2+} e^{i\Omega t} + \Omega- A_{2-} e^{-i\Omega t} \right)
\]

The initial state is 
\[
|\psi(0)\rangle = |z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a(0) \\ b(0) \end{pmatrix} = \begin{pmatrix} \alpha(0) \\ \beta(0) \end{pmatrix}
\]

Therefore, 
\[
0 = A_{2+} + A_{2-} \\
1 = \frac{2}{\omega_1} (\Omega+ A_{2+} + \Omega- A_{2-})
\]

or 
\[
A_{2+} = -A_{2-} = \frac{1}{2} \frac{\omega_1}{\Omega_+ - \Omega_-} = \frac{\omega_1}{2\Omega}
\]
so that

\[ b(t) = \beta(t)e^{-i\omega_0 t/2} = e^{-i\omega_0 t/2}A_2^{+}\left(e^{i\Omega t/2} - e^{-i\Omega t/2}\right) \]

\[ = e^{-i\omega_0 t/2}e^{i\omega_0 t/2}A_2^{+}\left(e^{i\Omega t/2} - e^{-i\Omega t/2}\right) \]

\[ = e^{-i\omega_0 t/2}e^{i\omega_0 t/2}i\omega_1 \Omega \left(i\sin\frac{\Omega t}{2}\right) \]

Finally,

\[ P = |b(t)|^2 = \left|e^{-i\omega_0 t/2}e^{i\omega_0 t/2}i\omega_1 \Omega \left(i\sin\frac{\Omega t}{2}\right)\right|^2 = \frac{\omega_1^2}{\Omega^2} \sin^2\frac{\Omega t}{2} \]

as in the earlier discussion.

9.7.24 More addition of angular momentum

Consider a system of two particles with \( j_1 = 2 \) and \( j_2 = 1 \). Determine the \(|j,m,j\rangle\) states listed below in the \(|j_1,m_1,j_2\rangle\) basis.

\(|3,3,j_1,j_2\rangle, |3,2,j_1,j_2\rangle, |3,1,j_1,j_2\rangle, |2,2,j_1,j_2\rangle, |2,1,j_1,j_2\rangle, |1,1,j_1,j_2\rangle\)

We have \( 2 \otimes 1 = 1 \oplus 2 \oplus 3 \). Now in the \(|m_1,m_2\rangle\) basis

\( j_1 = 2 \rightarrow m_1 = \pm 2, \pm 1, 0 \rightarrow 5 \) states and \( j_2 = 1 \rightarrow m_2 = \pm 1, 0 \rightarrow 3 \) states

so that we have a total of \( 5 \times 3 = 15 \) states.

Similarly, in the \(|J,M\rangle\) basis

\( J = 3 \rightarrow M = \pm 3, \pm 2, \pm 1, 0 \rightarrow 7 \) states
\( J = 2 \rightarrow M = \pm 2, \pm 1, 0 \rightarrow 5 \) states
\( J = 1 \rightarrow M = \pm 1, 0 \rightarrow 3 \) states

for a total of \( 7 + 5 + 3 = 15 \) states.

We now use Clebsch-Gordon coefficients technology to construct the \(|J,M\rangle\) states from the \(|m_1,m_2\rangle\) states.

Remember

\[ J_+ |j,m\rangle = \hbar\sqrt{j(j+1) - m(m-1)} |j,m\rangle \]

The highest \(|J,M\rangle\) is \(|3,3\rangle = |2,1\rangle_m\). Therefore,

\[ J_- |3,3\rangle = \sqrt{6}\hbar |3,2\rangle = (J_1_- + J_2_-) |2,1\rangle_m = 2\hbar |1,1\rangle_m + \sqrt{2}\hbar |2,0\rangle_m \]

\( \rightarrow |3,2\rangle = \frac{\sqrt{2}}{3} |1,1\rangle_m + \frac{\sqrt{3}}{3} |2,0\rangle_m \)
and

\[ J_- |3, 2\rangle = \sqrt{10} \hbar |3, 1\rangle = (J_{1-} + J_{2-}) \left( \sqrt{\frac{2}{3}} |1, 1\rangle_m + \sqrt{\frac{4}{3}} |2, 0\rangle_m \right) \]

\[ = \sqrt{\frac{2}{3}} \sqrt{6} \hbar |0, 1\rangle_m + \sqrt{\frac{1}{3}} 2 \hbar |1, 0\rangle_m + \sqrt{\frac{2}{3}} \sqrt{2} \hbar |1, 0\rangle_m + \frac{1}{3} \sqrt{2} \hbar |2, -1\rangle_m \]

\[ \rightarrow |3, 1\rangle = \sqrt{\frac{8}{15}} |1, 0\rangle_m + \sqrt{\frac{2}{5}} |0, 1\rangle_m + \frac{1}{15} |2, -1\rangle_m \]

Now

\[ |2, 2\rangle = a |1, 1\rangle_m + b |2, 0\rangle_m \quad , \quad a^2 + b^2 = 1 \]

and

\[ \langle 3, 2 | 2, 2 \rangle = 0 = \sqrt{\frac{2}{3}} a + \sqrt{\frac{1}{3}} b \]

which gives

\[ b = -\sqrt{2} a \rightarrow a = \sqrt{\frac{1}{3}} \rightarrow b = -\sqrt{\frac{2}{3}} \]

so that

\[ |2, 2\rangle = \sqrt{\frac{1}{3}} |1, 1\rangle_m - \frac{\sqrt{2}}{3} |2, 0\rangle_m \]

Then

\[ J_- |2, 2\rangle = 2 \hbar |2, 1\rangle = (J_{1-} + J_{2-}) \left( \sqrt{\frac{1}{3}} |1, 1\rangle_m - \frac{2}{3} |2, 0\rangle_m \right) \]

\[ = \sqrt{\frac{1}{3}} \sqrt{6} \hbar |0, 1\rangle_m - \frac{1}{3} 2 \hbar |1, 0\rangle_m + \sqrt{\frac{1}{3}} \sqrt{2} \hbar |1, 0\rangle_m - \frac{2}{3} \sqrt{2} \hbar |2, -1\rangle_m \]

\[ \rightarrow |2, 1\rangle = \sqrt{\frac{1}{2}} |0, 1\rangle_m - \sqrt{\frac{1}{6}} |1, 0\rangle_m - \frac{1}{3} |2, -1\rangle_m \]

Finally,

\[ |1, 1\rangle = a |0, 1\rangle_m + b |1, 0\rangle_m + c |2, -1\rangle_m \quad , \quad a^2 + b^2 + c^2 = 1 \]

and

\[ \langle 2, 1 | 1, 1 \rangle = 0 = \sqrt{\frac{2}{3}} a - \sqrt{\frac{1}{3}} b - \sqrt{\frac{1}{3}} c \]

\[ \langle 3, 1 | 1, 1 \rangle = 0 = \sqrt{\frac{2}{5}} a + \sqrt{\frac{2}{5}} b + \sqrt{\frac{1}{15}} c \]

so that

\[ c = \sqrt{6} a \quad , \quad b = -\sqrt{3} a \]

\[ a = \sqrt{\frac{1}{10}} \rightarrow b = -\sqrt{\frac{2}{10}} \quad , \quad c = \sqrt{\frac{3}{5}} \]

and

\[ |1, 1\rangle = \sqrt{\frac{1}{10}} |0, 1\rangle_m - \sqrt{\frac{3}{10}} |1, 0\rangle_m + \sqrt{\frac{3}{5}} |2, -1\rangle_m \]

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9.7.25 Clebsch-Gordan Coefficients

Work out the Clebsch-Gordan coefficients for the combination

\[ \frac{3}{2} \otimes \frac{1}{2} \]

We have that

\[ \frac{3}{2} \otimes \frac{1}{2} = 1 \oplus 2 \]

The maximum state is \( |j = 1, m = 2 \rangle = |2, 2 \rangle \) which is written as \( |2, 2 \rangle = |\frac{3}{2}, \frac{3}{2} \rangle |\frac{1}{2}, \frac{1}{2} \rangle \). From the general formula for ladder operators we have

\[ J_{\pm} |j, m \rangle = \sqrt{j(j + 1) - m(m \pm 1)} |j, m \pm 1 \rangle \]

where we have chosen \( \hbar = 1 \) for convenience. We then have

\[ J_{-} |2, 2 \rangle = 2 |2, 1 \rangle = (J^{a} + J^{b}) (|\frac{3}{2}, \frac{3}{2} \rangle |\frac{1}{2}, \frac{1}{2} \rangle) = \sqrt{3} |\frac{3}{2}, \frac{1}{2} \rangle |\frac{1}{2}, \frac{1}{2} \rangle + |\frac{3}{2}, \frac{3}{2} \rangle |\frac{1}{2}, -\frac{1}{2} \rangle \]

\[ \rightarrow |2, 1 \rangle = \frac{\sqrt{3}}{2} |\frac{3}{2}, \frac{1}{2} \rangle |\frac{1}{2}, \frac{1}{2} \rangle + \frac{1}{2} |\frac{3}{2}, \frac{3}{2} \rangle |\frac{1}{2}, -\frac{1}{2} \rangle \]

and

\[ J_{-} |2, 1 \rangle = \sqrt{6} |2, 0 \rangle = (J^{a} + J^{b}) \left( \frac{\sqrt{3}}{2} |\frac{3}{2}, \frac{1}{2} \rangle |\frac{1}{2}, \frac{1}{2} \rangle + \frac{1}{2} |\frac{3}{2}, \frac{3}{2} \rangle |\frac{1}{2}, -\frac{1}{2} \rangle \right) \]

\[ = \frac{\sqrt{3}}{2} |\frac{3}{2}, -\frac{1}{2} \rangle |\frac{1}{2}, \frac{1}{2} \rangle + \frac{\sqrt{3}}{2} |\frac{3}{2}, \frac{1}{2} \rangle |\frac{1}{2}, -\frac{1}{2} \rangle + \frac{\sqrt{3}}{2} |\frac{3}{2}, \frac{3}{2} \rangle |\frac{1}{2}, -\frac{1}{2} \rangle \]

\[ \rightarrow |2, 0 \rangle = \frac{1}{\sqrt{2}} |\frac{3}{2}, -\frac{1}{2} \rangle |\frac{1}{2}, \frac{1}{2} \rangle + \frac{1}{\sqrt{2}} |\frac{3}{2}, \frac{1}{2} \rangle |\frac{1}{2}, -\frac{1}{2} \rangle \]

Similarly,

\[ |2, -1 \rangle = \frac{\sqrt{3}}{2} |\frac{3}{2}, -\frac{1}{2} \rangle |\frac{1}{2}, -\frac{1}{2} \rangle + \frac{1}{2} |\frac{3}{2}, -\frac{3}{2} \rangle |\frac{1}{2}, \frac{1}{2} \rangle \]

and

\[ |2, -2 \rangle = |\frac{3}{2}, -\frac{3}{2} \rangle |\frac{1}{2}, -\frac{1}{2} \rangle \]

To find the \( |1, m \rangle \) states we start with \( |1, 1 \rangle \) which must be a linear combination

\[ |1, 1 \rangle = a \left( \frac{3}{2}, \frac{1}{2} \right) \left( \frac{3}{2}, \frac{1}{2} \right) + b \left( \frac{3}{2}, \frac{3}{2} \right) \left( \frac{1}{2}, -\frac{1}{2} \right) \]

with

\[ a^{2} + b^{2} = 1 \] and \( \langle 1, 1 \mid 2, 1 \rangle = 0 = \frac{\sqrt{3}}{2} a + \frac{1}{2} b \]

or

\[ b = -\frac{\sqrt{3}}{2} a \rightarrow 4a^{2} = 1 \rightarrow a = \frac{1}{2} \rightarrow b = -\frac{\sqrt{3}}{2} \]

so that

\[ |1, 1 \rangle = \frac{1}{2} \left( \frac{3}{2}, \frac{1}{2} \right) \left( \frac{3}{2}, \frac{1}{2} \right) - \frac{\sqrt{3}}{2} \left( \frac{3}{2}, \frac{3}{2} \right) \left( \frac{1}{2}, -\frac{1}{2} \right) \]

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Using the same procedure as above we find

\[
|1, 0\rangle = \frac{1}{\sqrt{2}} |\frac{3}{2}, \frac{1}{2}\rangle^a |\frac{1}{2}, -\frac{1}{2}\rangle^b - \frac{1}{\sqrt{2}} |\frac{3}{2}, -\frac{1}{2}\rangle^a |\frac{1}{2}, \frac{1}{2}\rangle^b
\]

\[
|1, -1\rangle = -\frac{1}{\sqrt{2}} |\frac{3}{2}, -\frac{1}{2}\rangle^a |\frac{1}{2}, \frac{1}{2}\rangle^b + \frac{1}{\sqrt{2}} |\frac{3}{2}, -\frac{1}{2}\rangle^a |\frac{1}{2}, -\frac{1}{2}\rangle^b
\]

All states are automatically normalized to unity and all orthogonality relations are satisfied.

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 \(\gamma\) 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

\[
\langle A \rangle = Tr \left( \hat{\rho} A \right)
\]

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.
Let us consider the \( i^{th} \) component of the polarization

\[
\frac{i}{\hbar} \frac{dP_i}{dt} = \frac{i}{\hbar} \frac{d\langle \sigma_i \rangle}{dt} = \frac{i}{\hbar} \frac{d}{dt} \text{Tr}(\rho \sigma_i) = \frac{i}{\hbar} \text{Tr}(\frac{\partial \rho}{\partial t} \sigma_i)
\]

\[
= \text{Tr}(\hat{H}, \rho \sigma_i) = \text{Tr}(\hat{H} \rho \sigma_i - \rho \hat{H} \sigma_i) = \text{Tr}(\sigma_i \hat{H} \rho - \hat{H} \sigma_i \rho) = \text{Tr}(\sigma_i \hat{H} \rho)
\]

\[
= -\text{Tr}(\sigma_i, \vec{\mu} \cdot \vec{B}) \hat{\rho} = \frac{1}{2} \gamma \text{Tr} \left( \sigma_i \sum_{j=1}^{3} \hat{\sigma}_j B_j \right) \hat{\rho}
\]

\[
= -\frac{1}{2} \gamma \sum_{j=1}^{3} B_j \text{Tr}(\hat{\sigma}_i, \hat{\sigma}_j) \hat{\rho}
\]

To proceed further, we need the density matrix for a state with polarization \( \vec{P} \).

Since \( \hat{\rho} \) is hermitian, it must be of the form

\[
\hat{\rho} = a(\hat{I} + \vec{b} \cdot \vec{\sigma})
\]

that is, \( \{\hat{I}, \vec{\sigma}\} \) are a basis set for all \( 2 \times 2 \) matrices. But its trace must be one, so that

\[
\text{Tr} \hat{\rho} = 1 = a(\text{Tr} \hat{I} + \text{Tr}(\vec{b} \cdot \vec{\sigma})) = a(2 + 0) \Rightarrow a = 1/2
\]

Finally, to get the right polarization vector, we must have

\[
\text{Tr} (\hat{\rho} \vec{\sigma}) = \langle \vec{\sigma} \rangle = \vec{P} = a(\text{Tr} \vec{\sigma} + \text{Tr} ((\vec{b} \cdot \vec{\sigma}) \vec{\sigma}))
\]

\[
= \frac{1}{2} (0 + \text{Tr} ((\vec{b} \cdot \vec{\sigma}) \vec{\sigma})) = \frac{1}{2} \text{Tr} ((\vec{b} \cdot \vec{\sigma}) \vec{\sigma})
\]

Now

\[
\vec{b} \cdot ((\vec{b} \cdot \vec{\sigma}) \vec{\sigma}) = (\vec{b} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = \vec{b} \cdot \vec{b} + i \vec{\sigma} \cdot \vec{b} \times \vec{b} = \vec{b} \cdot \vec{b}
\]

or

\[
(\vec{b} \cdot \vec{\sigma}) \vec{\sigma} = \vec{b}
\]

so that

\[
\vec{P} = \text{Tr} (\hat{\rho} \vec{\sigma}) = \frac{1}{2} \text{Tr} ((\vec{b} \cdot \vec{\sigma}) \vec{\sigma}) = \frac{1}{2} \text{Tr} \hat{I} = \vec{b}
\]

Thus, we have

\[
\frac{i}{\hbar} \frac{dP_i}{dt} = \frac{1}{4} \gamma \sum_{j=1}^{3} B_j \left( \text{Tr}((\hat{\sigma}_i, \hat{\sigma}_j)) + \sum_{k=1}^{3} P_k \text{Tr}(\hat{\sigma}_i, \hat{\sigma}_j \hat{\sigma}_k) \right)
\]

Now \( [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\varepsilon_{ijk} \hat{\sigma}_k \), which is traceless. Further,

\[
\text{Tr}((\hat{\sigma}_i, \hat{\sigma}_j) \hat{\sigma}_k) = 2i\varepsilon_{ijk} \text{Tr}(\hat{\sigma}_k \hat{\sigma}_k) = 4i\varepsilon_{ijk}
\]
This gives the result
\[
\frac{dP_i}{dt} = -\gamma \sum_{j=1}^{3} \sum_{k=1}^{3} \varepsilon_{ijk} B_j P_k
\]
or
\[
\frac{d\vec{P}}{dt} = \gamma \vec{P} \times \vec{B}
\]
which implies that \( \vec{P} \) precesses about the direction of \( \vec{B} \).

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 \( \vec{M} = N\gamma \langle \sigma \rangle / 2 \) (dont work too hard to evaluate).

Let us orient our coordinate system so that the \( z \)-axis is along the magnetic field direction. The \( M_x = M_y = 0 \), and
\[
M_z = N\gamma \frac{1}{2} \langle \sigma_z \rangle = N\gamma \frac{1}{2Z} Tr \left( e^{-\hat{H}/T} \sigma_z \right)
\]
where \( H = -\gamma B_z \sigma_z / 2 \).

(b) What is the magnetization in the high-temperature limit, to lowest nontrivial order (this I want you to evaluate as completely as you can!)?

In the high temperature limit, we will discard terms of order higher than \( 1/T \) in the expansion of the exponential, i.e.,
\[
e^{-\hat{H}/T} \approx 1 - \frac{H}{T} = 1 + \gamma B_z \frac{1}{2T}
\]
Thus,
\[
M_z = N\gamma \frac{1}{2Z} Tr \left( \left( 1 + \gamma B_z \frac{1}{2T} \right) \sigma_z \right) = N\gamma^2 B_z \frac{1}{2ZT}
\]
Furthermore,
\[ Z = Tr \left( e^{-H/T} \right) = 2 + O(1/T^2) \]
so we have the result
\[ M_z = \frac{N\gamma^2 B_z}{4T} \]

This is referred to as the Curie Law for magnetization of a system of spin-1/2 particles.

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 \(\langle \hat{L}^2 \rangle\), \(\langle \hat{L}_x \rangle\) and \(\langle \hat{L}_z \rangle\)?

\[ \langle E \rangle = E_1 P(E_1) + E_2 P(E_2) = \left( \frac{4}{5} \right)^2 \left( -\frac{1}{2}\mu e^2 \alpha^2 \right) + \left( \frac{3}{5} \right)^2 \left( -\frac{1}{2}\mu e^2 \alpha^2 \right) = -\frac{73}{250}\mu e^2 \alpha^2 \]
\[ \langle \hat{L}^2 \rangle = (L^2) P((L^2)_{1}) + (L^2) P((L^2)_{2}) = \left( \frac{4}{5} \right)^2 (0) + \left( \frac{3}{5} \right)^2 (2\hbar^2) = \frac{18}{25}\hbar^2 \]
\[ \langle \hat{L}_z \rangle = (L_z) P((L_z)_{1}) + (L_z) P((L_z)_{2}) = \left( \frac{4}{5} \right)^2 (0) + \left( \frac{3}{5} \right)^2 (\hbar) = \frac{9}{25}\hbar \]

(b) What is \(|\psi(t)\rangle\)? Which, if any, of the expectation values in (a) vary with time?

Now
\[ |\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = \frac{4}{5} e^{-iE_1t/\hbar} |1,0,0\rangle + \frac{3i}{5} e^{-iE_2t/\hbar} |2,1,1\rangle \]

Since
\[ \left[ \hat{H}, \hat{H} \right] = \left[ \hat{H}, \hat{L}^2 \right] = \left[ \hat{H}, \hat{L}_z \right] = 0 \]
and
\[ \frac{d\langle A \rangle}{dt} = \frac{i}{\hbar} \langle \psi | \left[ \hat{H}, \hat{A} \right] |\psi\rangle \]
all expectation values are independent of 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)?
The classical turning point occurs when the kinetic energy is zero, that is, when the total energy equals the potential energy. Therefore,

\[-\frac{e^2}{r_+} = E_1 = -\frac{1}{2} \mu c^2 \alpha^2 \rightarrow r_+ = \frac{2e^2}{\mu c^2 \alpha^2} = \frac{2\hbar}{\mu c \alpha} = 2a_0\]

Now for the ground state

\[R_{10}(r) = 2 \left( \frac{1}{a_0} \right)^{3/2} e^{-r/a_0}\]

and the probability of being outside the classical turning point is

\[P(r \geq r_+) = \int_0^{2a_0} R_{10}^2(r) r^2 dr = \frac{4}{a_0^3} \int_0^{2a_0} e^{-2r/a_0} r^2 dr\]

\[= \frac{4}{a_0^3} \left[ \frac{r^2 e^{-2r/a_0}}{(-2/a_0)} - \frac{2}{(-2/a_0)^2} e^{-2r/a_0} \left( -\frac{2r}{a_0} - 1 \right) \right]_{r=2a_0}^{r=\infty}\]

\[= 4e^{-4} \left[ 2a_0^3 + \frac{5}{4} a_0^3 \right] = 13e^{-4} = 0.24\]

(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.

Now

\[R_{10}(r) = 2 \left( \frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}\]

For tritium in the ground state we have

\[|initial\rangle = |1, 0, 0; Z = 1\rangle\]
\[|final\rangle = |1, 0, 0; Z = 2\rangle\]

Therefore,

\[(final \mid initial) = \int d^3r \langle final \mid \vec{r} \rangle \langle \vec{r} \mid initial\rangle = \int_0^{\infty} R_{10}^{Z=2} R_{10}^{Z=1} r^2 dr\]

\[= \frac{4}{a_0^2} 2^{3/2} \int_0^{\infty} e^{-3r/a_0} r^2 dr = \frac{8^{3/2}}{3^3}\]

Therefore,

\[P(remain) = |(final \mid initial)|^2 = \left[ \frac{8^{3/2}}{3^3} \right]^2 = \frac{64 \cdot 8}{(27)^2} = 0.70\]
9.7.30 What happens?

At the time \( t = 0 \) the wave function for the hydrogen atom is

\[
\psi(\vec{r}, 0) = \frac{1}{\sqrt{10}} \left( 2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{211} \right)
\]

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?

\[
\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle = \sum_n E_n P(E_n) = \frac{1}{10} (4E_1 + E_2 + 2E_2 + 3E_2)
\]

\[
= \frac{1}{5} (2E_1 + 3E_2) = 0.55E_1 = -0.55(13.6) = -7.47 \text{ eV}
\]

(b) What is the probability of finding the system with \( \ell = 1, m = +1 \) as a function of time?

\[
P_{11}(t) = \langle 2, 1, 1 | \psi(t) \rangle^2 = \left| \langle 2, 1, 1 | e^{-i\hat{H}t/\hbar} | \psi(0) \rangle \right|^2
\]

\[
= \left| \langle 2, 1, 1 | \left( \frac{1}{\sqrt{10}} \left( 2e^{-iE_1t/\hbar} |1, 0, 0\rangle + e^{-iE_2t/\hbar} |2, 1, 0\rangle \right) + \sqrt{2}e^{-iE_2t/\hbar} |2, 1, 1\rangle + \sqrt{3}e^{-iE_2t/\hbar} |2, 1, -1\rangle \right) \right|^2
\]

\[
= \frac{1}{5}
\]

(c) What is the probability of finding an electron within \( 10^{-10} \text{ cm} \) of the proton (at time \( t = 0 \))? A good approximate result is acceptable.

Let \( \alpha = 10^{-10} \text{ cm} \). Then we have

\[
P(r < \alpha; t = 0) = \int_0^\alpha \int \psi^*(0)\psi(0)r^2 drd\Omega = \frac{1}{10} \int_0^\alpha (4R_{10}^2 + 6R_{21}^2)r^2 dr
\]

where

\[
R_{10}^2 = \frac{4}{a^3} e^{-2r/a}, \quad R_{21}^2 = \frac{r^2}{24a^5} e^{-r/2a}, \quad a = a_0 = 5.29 \times 10^{-9} \text{ cm}
\]

Since \( r \leq \alpha << a \) we can make approximations

\[
R_{10}^2 = \frac{4}{a^3} \left( 1 - \frac{2r}{a} \right), \quad R_{21}^2 = \frac{r^2}{24a^5} \left( 1 - \frac{r}{2a} \right)
\]
Therefore,

\[
P(r < \alpha; t = 0) = \frac{4}{10} \int_0^\alpha \left(1 - \frac{2r}{a}\right) r^2 dr + \frac{6}{10} \frac{1}{24a^5} \int_0^\alpha \left(1 - \frac{r}{2a}\right) r^4 dr
\]

\[
= \frac{4}{10} \left[ \frac{4}{3} \left(\frac{\alpha}{a}\right)^3 - 2 \left(\frac{\alpha}{a}\right)^4 \right] + \frac{6}{10} \left[ \frac{1}{120} \left(\frac{\alpha}{a}\right)^5 - \frac{1}{288} \left(\frac{\alpha}{a}\right)^6 \right]
\]

\[
\approx \frac{8}{15} \left(\frac{\alpha}{a}\right)^3 = 3.6 \times 10^{-6}
\]

(d) Suppose a measurement is made which shows that \( L = 1, \ L_x = +1 \). Determine the wave function immediately after such a measurement.

Now a measurement gives \( L = 1, L_x = +1 \). Since \( n \geq L + 1 \), we have \( n = 2 \). Therefore, after the measurement

\[
|\psi\rangle = C_0 |2, 1, 0\rangle + C_+ |2, 1, 1\rangle + C_- |2, 1, -1\rangle
\]

Since the measurement gave \( L_x = +1 \), the collapse postulate says that we must have

\[
\hat{L}_x |\psi\rangle = C_0 \hat{L}_x |2, 1, 0\rangle + C_+ \hat{L}_x |2, 1, 1\rangle + C_- \hat{L}_x |2, 1, -1\rangle
\]

\[
= |\psi\rangle = C_0 |2, 1, 0\rangle + C_+ |2, 1, 1\rangle + C_- |2, 1, -1\rangle
\]

\[
\rightarrow \frac{1}{2} \left( \sqrt{2} C_0 |2, 1, 1\rangle + \sqrt{2} (C_+ + C_-) |2, 1, 0\rangle + \sqrt{2} C_0 |2, 1, -1\rangle \right)
\]

\[
= C_0 |2, 1, 0\rangle + C_+ |2, 1, 1\rangle + C_- |2, 1, -1\rangle
\]

\[
\rightarrow C_+ = \frac{C_0}{\sqrt{2}} \rightarrow |\psi\rangle = \frac{1}{2} C_0 \left( 2 |2, 1, 0\rangle + \sqrt{2} |2, 1, 1\rangle + \sqrt{2} |2, 1, -1\rangle \right)
\]

Normalizing gives \( C_0 = 1/\sqrt{2} \) so that

\[
|\psi\rangle = \frac{1}{2} \left( \sqrt{2} |2, 1, 0\rangle + |2, 1, 1\rangle + |2, 1, -1\rangle \right)
\]

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?
The eigenvectors of the Hamiltonian in configuration space are
\[ \psi_{n_1n_2n_3}(x_1, x_2, x_3) = e^{-\frac{1}{2} \frac{m \omega_1}{\hbar} x_1^2} H_{n_1} \left( \sqrt{\frac{m \omega_1}{\hbar}} x_1 \right) e^{-\frac{1}{2} \frac{m \omega_2}{\hbar} x_2^2} H_{n_2} \left( \sqrt{\frac{m \omega_2}{\hbar}} x_2 \right) \]
\[ \times e^{-\frac{1}{2} \frac{m \omega_3}{\hbar} x_3^2} H_{n_3} \left( \sqrt{\frac{m \omega_3}{\hbar}} x_3 \right) \]
with
\[ \omega_0 = \omega_1 = \omega_2 = \omega \sqrt{1 - \tau}, \quad \omega_3 = \omega \sqrt{1 + \tau} \]

The corresponding energy eigenvalues are
\[ E(n_1, n_2, n_3) = \hbar \omega_0 (n_1 + n_2 + 1) + \hbar \omega_3 (n_3 + 1/2) \]

(b) Calculate and discuss, as functions of \( \tau \), the variation of the energy and the degree of degeneracy of the ground state and the first two excited states.

For generic values of \( \tau \), the degeneracy is the same as that of the 2-dimensional oscillator. In fact, we can write
\[ E(n, n_3) = E(n_1, n_2, n_3) = \hbar \omega_0 (n - n_3 + 1) + \hbar \omega_3 (n_3 + 1/2) \]
where \( n = n_1 + n_2 + n_3 \). For given \( n \) and \( n_3 \) all the eigenvectors with \( n_1 = 0, 1, 2, \ldots, n - n_3 \) have the same energy, so the degeneracy is \( n - n_3 + 1 \). The ground state corresponds to \( n = 0 = n_3 \), so this state is not degenerate.

For \( n = 1 \), there are two different energy levels,
\[ E(1, 0) = 2 \hbar \omega \sqrt{1 - \tau} + \frac{1}{2} \hbar \omega \sqrt{1 + \tau} \]
\[ E(1, 1) = \hbar \omega \sqrt{1 - \tau} + \frac{3}{2} \hbar \omega \sqrt{1 + \tau} \]

\( E(1, 0) \) has degeneracy 2, while \( E(1, 1) \) is not degenerate. Since
\[ E(1, 1) - E(1, 0) = \hbar \omega (\sqrt{1 + \tau} - \sqrt{1 - \tau}) > 0 \]
for \( \tau > 0 \), it follows that
\[ E(0, 0) < E(1, 0) < E(1, 1) \]

For special values of \( \tau \), the degeneracies can be accidentally higher. For example, if \( \tau = 0 \) we have an isotropic 3-dimensional oscillator and the energy levels depend only on \( n \) and the degeneracy of the \( n \)th level is \( (n+1)(n+2)/2 \). Then \( E(1, 1) = E(1, 0) \) and this level is triply degenerate.

There are other values of \( \tau \) for which degeneracies are higher than the generic values. For examples, for \( \tau = 3/5 \),
\[ \sqrt{1 + \tau} = 2 \sqrt{1 - \tau} \]
and then
\[ E(n, n_3) = \hbar \omega (n + n_3 + 2) \sqrt{1 - \tau} \]

In this case
\begin{align*}
E(0, 0) &= 2\hbar \omega \sqrt{1 - \tau} \\
E(1, 0) &= 3\hbar \omega \sqrt{1 - \tau} \\
E(1, 1) &= 4\hbar \omega \sqrt{1 - \tau}
\end{align*}

so the levels remain separated. However, for \( n = 2 \), we have the levels
\begin{align*}
E(2, 0) &= 4\hbar \omega \sqrt{1 - \tau} \\
E(2, 1) &= 5\hbar \omega \sqrt{1 - \tau} \\
E(2, 2) &= 6\hbar \omega \sqrt{1 - \tau}
\end{align*}

so that the three eigenvectors corresponding to \( E(2, 0) \) are degenerate with the eigenvector corresponding to \( E(1, 1) \). The energy level is thus quadruply degenerate for this particular value of \( \tau \).

Evidently, similar coincidental degeneracies occur whenever \( \tau \) is such that
\[ \sqrt{1 + \tau} = N \sqrt{1 - \tau} \]
with \( N \) a positive integer.

### 9.7.32 Exponential potential

Two particles, each of mass \( M \), are attracted to each other by a potential
\[ V(r) = -\left( \frac{\gamma^2}{d} \right) e^{-r/d} \]
where \( d = \hbar/mc \) with \( mc^2 = 140 \text{ MeV} \) and \( Mc^2 = 940 \text{ MeV} \).

(a) Show that for \( \ell = 0 \) the radial Schrödinger 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 \( \alpha \) and \( \beta \).

When \( \ell = 0 \), the radial wave function \( R(r) = \chi(r)/r \) satisfies the equation
\[ \frac{d^2 \chi}{dr^2} + \frac{M}{\hbar^2} \left( E + \frac{\gamma^2}{d} e^{-r/d} \right) \chi = 0 \]
where \( \mu = M/2 \) is the reduced mass.

Now, changing variables: \( r \to x = \alpha e^{-\beta r} \), \( x \in [0, \alpha] \) and writing \( \chi(r) = J(x) \) we get
\[ \frac{d}{dr} = \frac{dx}{dr} \frac{d}{dx} = -\beta \alpha e^{-\beta r} \frac{d}{dx} = -\beta x \frac{d}{dx} \]
\[ \frac{d^2}{dr^2} = \frac{dx}{dr} \frac{d}{dx} \left( \frac{d}{dx} \right) = \frac{dx}{dr} \frac{d}{dx} \left( -\beta x \frac{d}{dx} \right) = -\beta x \left( -\beta \frac{d}{dx} - \beta x \frac{d^2}{dx^2} \right) \]
Therefore,
\[-\beta x \left( -\beta \frac{d}{dx} - \beta x \frac{d^2}{dx^2} \right) J(x) + \frac{M}{\hbar} \left( E + \frac{g^2}{\hbar} \left( \frac{x}{a} \right)^{1/d\beta} \right) J(x) = 0\]
\[
\frac{d^2 J}{dx^2} + \frac{1}{x} \frac{dJ}{dx} + \frac{M}{\beta \hbar^2 x^2} \left( E + \frac{g^2}{\hbar} \left( \frac{x}{a} \right)^{1/d\beta} \right) J = 0
\]
We now choose
\[\alpha = \frac{2g}{\hbar} \sqrt{Md}, \quad \beta = \frac{1}{2d}, \quad \rho^2 = \frac{4d^2 M |E|}{\hbar^2}\]
so that the equation becomes Bessel’s equation of order \(\rho\)
\[
\frac{d^2 J_\rho(x)}{dx^2} + \frac{1}{x} \frac{dJ_\rho(x)}{dx} + \left( 1 - \frac{\rho^2}{x^2} \right) J_\rho(x) = 0
\]
The solution (unnormalized) is
\[R(r) = \frac{\chi(r)}{r} = \frac{J_\rho(\alpha e^{-\beta r})}{r}\]

(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.

For bound states we require
\[\lim_{r \to \infty} R(r) \to 0 \Rightarrow J_\rho \text{ remains finite or } \rho \geq 0\]
\[R(r) \text{ must also be finite at } r = 0, \text{ which means that } \chi(0) = J_\rho(\alpha) = 0.\]
This equation has an infinite number of real roots.

For
\[E = 2.2 \text{ MeV}, \quad \rho = \frac{2d}{\hbar} \sqrt{M |E|} = \frac{2}{mc^2} \sqrt{Mc^2 |E|} = \frac{2}{140} \sqrt{940 \cdot 2.2} \approx 0.65\]
The graph below shows some contours of \(J_\rho(\alpha)\) for different values of the function in the \(\alpha - \rho\) plane. The values are indicated by the contour markers (see MATLAB code below).

MATLAB code:

n=0.05*(0:40);x=0.05*(0:160);
nx=length(x);nn=length(n);
ox=ones(1,nx);xxx=x(:)*ox(:)';
on=ones(1,nx);nnn=on(:)*n(:)';
zz=besselj(nnn,xxx);
figure
[C,h]=contour(nnn,xxx,zz,[-0.3,-0.2,-0.1,0.0,0.1,0.2,0.3],'k');
Figure 9.2: $J_\rho(\alpha)$ contours in the $\alpha - \rho$ plane
The lowest zero of $J_\rho(\alpha)$ for $\rho = 0.65$ is $\alpha = 3.3$. This corresponds to the intersection of the vertical (dashed) line from $\rho = 0.65$ and the 0.0 contour. The next intersection is $\alpha = 6.6$.

Thus, for $\alpha = 3.3$, the system has only one $\ell = 0$ bound state, for which

$$\frac{g^2}{\hbar c} = \frac{\hbar \alpha^2}{4Mc} = \frac{\hbar mc^2\alpha^2}{4Mc^2} \approx 0.41 \text{ (dimensionless)}$$

(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 above.

For $\alpha = 6.6$, there is an additional $\ell = 0$ bound state. Thus, the minimum value of $\alpha$ for two $\ell = 0$ bound states is 6.6, for which

$$\frac{g^2}{\hbar c} = \frac{\hbar mc^2\alpha^2}{4Mc^2} \approx 1.62$$

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.

We consider an electron above an impenetrable conducting surface $(x, y, z)$ and its positive image charge $(x, -y, z)$ as the system. The potential
energy of the system is
\[ V(\vec{r}) = \frac{1}{2} \sum_i q_i V_i = \frac{1}{2} \left( (+e) \left( \frac{-e}{2y} \right) + (-e) \left( \frac{+e}{2y} \right) \right) = -\frac{e^2}{4y} \]

and the Schrödinger equation is then
\[ \left( -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4y} \right) \psi(x, y, z) = E \psi(x, y, z) \]

(b) What is the x and z dependence of the eigenstates?

Separating the variables we have
\[ \psi(x, y, z) = \psi_n(y) \varphi_x(x) \varphi_z(z) \]
\[ \frac{\hbar^2}{2m} \frac{d^2 \psi_n(y)}{dy^2} - \frac{e^2}{4y} \psi_n(y) = E \psi_n(y) \]
\[ \frac{\hbar^2}{2m} \frac{d^2 \varphi_x(x)}{dx^2} = \frac{p_x^2}{2m} \varphi_x(x) \quad \frac{\hbar^2}{2m} \frac{d^2 \varphi_z(z)}{dz^2} = \frac{p_z^2}{2m} \varphi_z(z) \]
\[ E = \frac{p_x^2}{2m} + \frac{p_z^2}{2m} + E_y \]

Note that since
\[ V(\vec{r}) = -\frac{e^2}{4y} \]

depends only on y, px and pz are constant of the motion. Therefore,
\[ \varphi_x(x) = e^{ip_x x/\hbar} \quad \varphi_z(z) = e^{ip_z z/\hbar} \]

so that
\[ \psi(x, y, z) = \psi_n(y) e^{i(p_x x + p_z z)/\hbar} \]

(c) What are the remaining boundary conditions?

The remaining boundary condition is
\[ \psi(x, y, z) = 0 \quad \text{for} \quad y \leq 0 \]

since that region is inside the conductor.

(d) Find the ground state and its energy? [HINT: they are closely related to those for the usual hydrogen atom]

Now consider a hydrogen-like atom of nuclear charge Z. The corresponding radial Schrödinger equation for \( R(r) = \chi(r)/r \) is
\[ -\frac{\hbar^2}{2m} \frac{d^2 \chi}{dr^2} - \frac{Ze^2}{r} \chi + \frac{\ell(\ell + 1)}{2mr^2} \chi = E \chi \]

Now, when \( \ell = 0 \), we have
\[ -\frac{\hbar^2}{2m} \frac{d^2 \chi}{dr^2} - \frac{Ze^2}{r} \chi = E \chi \]

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which is identical to the bouncing electron equation with the replacements

\[ r \rightarrow y, \quad Z \rightarrow \frac{1}{4} \]

Therefore, the solution for the bouncing electron ground states is

\[ \psi_1(y) = yR_{10}(y) = 2y \left( \frac{Z}{a} \right)^{3/2} e^{-Zy/a}, \quad a = \frac{\hbar^2}{me^2} \]

With \( Z = 1/4 \), we have

\[ \psi_1(y) = yR_{10}(y) = 2y \left( \frac{me^2}{4\hbar^2} \right)^{3/2} e^{-\frac{me^2}{4\hbar^2}y} \]

Note that the boundary condition (c) is satisfied by this wave function.

The ground state energy due to the \( y \)-motion is then

\[ E_y = -\frac{Z^2 me^4}{2\hbar^2} = -\frac{me^4}{32\hbar^2} \]

(e) What is the complete set of discrete and/or continuous energy eigenvalues?

The complete energy eigenvalue spectrum for the quantum state \( n \) is

\[ E_{n,p_x,p_z} = -\frac{me^4}{32\hbar^2} \frac{1}{n^2} + \frac{p_x^2}{2m} + \frac{p_z^2}{2m} \]

with wave function

\[ \psi_{n,p_x,p_z}(x,y,z) = A R_{n0}(y) e^{i(p_x x + p_z z)/\hbar} \]

where \( A \) is the normalization factor.

### 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 Schrödinger equation and calculate the energy levels.

The radial Schrödinger equation for the alkali atom is

\[ \frac{\hbar^2}{2m} \left( -\frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} \right) R_\ell(r) - \frac{e^2}{r} R_\ell(r) - \frac{e^2 b}{r^2} R_\ell(r) = E R_\ell(r) \]

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This can be rewritten as
\[ \frac{\hbar^2}{2m} \left( -\frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} \right) R_\ell(r) - \frac{e^2}{r} R_\ell(r) = E R_\ell(r) \]
where
\[ \ell(\ell + 1) = \ell(\ell + 1) - \beta e^2 \rightarrow \tilde{\ell} = -\frac{1}{2} + \sqrt{\ell(\ell + 1) - \beta e^2 + 1/4} \]
The rewritten equation is just the hydrogen atom with \( \ell \rightarrow \tilde{\ell} \).

The hydrogen atom has
\[ E = -\frac{e^2}{2a_0} \frac{1}{(k + \ell + 1)^2} \text{ with } k = 0, 1, 2, ..... \]
Therefore, we now define \( n = k + \ell + 1 \) as in the hydrogen atom solution and not \( n = k + \tilde{\ell} + 1 \), which would not be an integer. The alkali energy levels then become
\[ E = -\frac{e^2}{2a_0} \left( \frac{1}{n + \sqrt{(\ell + 1/2)^2 - \beta e^2 + 1/4} - \ell - 1/2} \right)^2 \]
Note that the energy levels depend on the angular momentum quantum number, \( \ell \), as well as the principal quantum number, \( n \). We need to restrict the parameter \( \beta e^2 \leq 1/4 \), to ensure that all these energy levels are real.

The accidental degeneracy of the hydrogen atom has been lifted.

**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.

The standard radial equation is
\[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \left( \frac{2m}{\hbar^2} (E - V(r)) - \frac{\ell(\ell + 1)}{r^2} \right) R = 0 \]
Substituting \( R(r) = \chi(r)/r \) we have
\[ \frac{d^2 \chi}{dr^2} + \left[ \frac{2m}{\hbar^2} (E - V(r)) - \frac{\ell(\ell + 1)}{r^2} \right] \chi = 0 \]
These equations are valid for \( a \leq r \leq b \).

For the ground state, \( \ell = 0 \). Using \( V(r) = 0 \) between the shells and letting \( K^2 = 2mE/\hbar^2 \), we have
\[ \frac{d^2 \chi}{dr^2} + K^2 \chi = 0 \text{ with } \chi(a) = \chi(b) = 0 \text{ (impermeable walls)} \]
The general solution is
\[ \chi(r) = A \sin Kr + B \cos Kr \]
\[ \chi(a) = 0 = A \sin Ka + B \cos Ka \Rightarrow \frac{B}{A} = -\tan Ka \]

We choose
\[ A = C \cos Ka, \quad B = -C \sin Ka \]

Therefore,
\[ \chi(r) = C(\cos Ka \sin Kr - \sin Ka \cos Kr) = C \sin K(r-a) \]

Now,
\[ \chi(b) = 0 = C \sin K(b-a) \Rightarrow K = \frac{n\pi}{b-a}, \quad n = 1, 2, 3,... \]

Normalization:
\[ \int_a^b r^2 R^2 dr = 1 = \int_a^b \chi^2 dr \Rightarrow C = \sqrt{\frac{2}{b-a}} \]

so that
\[ R_{10}(r) = \sqrt{\frac{2}{b-a}} \frac{1}{r} \sin \frac{\pi(r-a)}{b-a} \]

since ground state is \( n = 1 \)

Finally, the fully normalized wave function is
\[ \psi(\vec{r}) = R_{10}(r)Y_{00}(\Omega) = \frac{1}{\sqrt{4\pi}} \sqrt{\frac{2}{b-a}} \frac{1}{r} \sin \frac{\pi(r-a)}{b-a} \]

### 9.7.36 Logarithmic potential

A particle of mass \( m \) moves in the logarithmic potential
\[ V(r) = C \ln \left( \frac{r}{r_0} \right) \]

Show that:

(a) All the eigenstates have the same mean-squared velocity. Find this mean-squared velocity. Think Virial theorem!

We have
\[ \langle \dot{r}^2 \rangle = \frac{1}{m^2} \langle \dot{p}^2 \rangle = \frac{1}{m^2} \int d^3r \psi^*(\vec{r}) \dot{p}^2 \psi(\vec{r}) \]

For a stationary state, the virial theorem gives
\[ \langle T \rangle = \frac{1}{2} \langle \dot{r} \cdot \nabla V(\vec{r}) \rangle \]

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Therefore,\[
\langle \vec{v}^2 \rangle = \frac{1}{m^2} \langle \vec{p}^2 \rangle = \frac{2}{m} \langle T \rangle = \frac{1}{m} \langle \vec{r} \cdot \nabla V(\vec{r}) \rangle \quad \text{notag} \tag{9.2}
\]
\[
= \frac{1}{m} \int d^3r \frac{d}{dr} \left( C(\ell \nabla \cdot r) \right) \psi^* \psi = \frac{C}{m} \int d^3r \psi^* \psi = \frac{C}{m}
\]
which is true for any eigenstate.

(b) The spacing between any two levels is independent of the mass \(m\).

We have
\[
\frac{\partial E_n}{\partial m} = \frac{\partial \langle H \rangle}{\partial m} = \left\langle -\frac{\vec{p}^2}{2m^2} \right\rangle = -\frac{1}{2} \langle \vec{v}^2 \rangle = -\frac{C}{2m}
\]
This says that
\[
\frac{\partial E_n}{\partial m}
\]
is independent of \(n\) so that
\[
\frac{\partial (E_n - E_{n-1})}{\partial m} = -\frac{C}{2m} + \frac{C}{2m} = 0 \rightarrow E_n - E_{n-1}
\]
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 \(r_0\).

The attractive potential is represented by
\[
V(x) = \begin{cases} 
-V_0 & 0 \leq r \leq r_0 \\
0 & r > r_0
\end{cases}
\]

(a) What is the minimum depth of the potential needed to achieve two bound states of zero angular momentum? For a bound state \(0 > E > -V_0\). Therefore, for \(\ell = 0\), the radial wave function \(R(r) = \chi(r)/r\) satisfies the equations
\[
\frac{-\hbar^2}{2m} \frac{d^2\chi}{dr^2} - V_0\chi = E\chi \quad 0 \leq r \leq r_0
\]
\[
\frac{-\hbar^2}{2m} \frac{d^2\chi}{dr^2} = E\chi \quad r > r_0
\]
with boundary condition \(\chi(0) = 0\) and \(\chi(\infty) = \text{finite}\).

We can satisfy these conditions by choosing
\[
\chi(r) = \sin \alpha r \quad 0 \leq r \leq r_0
\]
\[
\chi(r) = Be^{-\beta r} \quad r > r_0
\]
where
\[ \alpha = \frac{1}{\hbar} \sqrt{2m(E + V_0)} \quad , \quad \beta = \frac{1}{\hbar} \sqrt{-2mE} \]

Now at \( r = r_j \), \( \chi(r) \) and \( d\chi/dr \) are continuous, so that
\[ \sin \alpha r_0 = B e^{-\beta r_0} \quad , \quad \alpha \cos \alpha r_0 = -B \beta e^{-\beta r_0} \]
which gives
\[ -\alpha \cot \alpha r_0 = \beta \]

Now defining \( \xi = \alpha r_0 \), \( \eta = \beta r_0 \) we have two equations defining the solutions corresponding to the energy eigenvalues
\[ \xi^2 + \eta^2 = \frac{2mV_0 r_0^2}{\hbar^2} \quad , \quad -\xi \cot \xi = \eta \]
Each set of positive numbers \( \xi \) and \( \eta \) satisfying these equations gives a bound state of the system.

We can solve the problem graphically as shown below.
We have plotted curves representing the equation
\[-\xi \cot \xi = \eta\]
and circles representing the equation
\[\xi^2 + \eta^2 = \frac{2mV_0r_0^2}{\hbar^2}\]
on an \(\xi - \eta\) plot.

Clearly from the plot, for a given value of \(V_0\), to have two intersections (2 bound states), the radius of the circle (there is only one circle for a given \(V_0\)) must be greater than \(3\pi/2\) or
\[
\frac{2mV_0r_0^2}{\hbar^2} \geq \left(\frac{3\pi}{2}\right)^2 \rightarrow V_0 \geq \frac{9\pi^2\hbar^2}{8mr_0^2}
\]
This is the minimum potential depth 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.

We have
\[
\xi^2 + \eta^2 = \left(\frac{3\pi}{2}\right)^2 \rightarrow \xi = \frac{3\pi}{2} \sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2}
\]
\[-\xi \cot \xi = \eta \rightarrow -\frac{3\pi}{2} \sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2} \cot \left(\frac{3\pi}{2} \sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2}\right) = \eta
\]
\[-\frac{2\eta}{3\pi} \tan \left(\frac{3\pi}{2} \sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2}\right) = \sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2}
\]
or
\[
f(\eta) = \sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2} + \frac{2\eta}{3\pi} \tan \left(\frac{3\pi}{2} \sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2}\right)
\]
\[= \sqrt{1 - 0.045\eta^2} + 0.212\eta \tan \left(4.712 \sqrt{1 - 0.045\eta^2}\right) = 0
\]
If we solve the last equation numerically (find the zeroes of \(f(\eta))\) to find \(\eta\), we get \(\eta = 0, 4.444\), and then the energy is given by
\[
\beta = \frac{\eta}{r_0}, \quad E = -\frac{\hbar^2}{2m} \beta^2 = -\frac{\hbar^2}{2mr_0^2} \eta^2
\]
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 \( \vec{E} = E_0 \hat{x} \).

(a) Solve for the complete energy spectrum.

We choose a gauge such that \( \vec{A} = B_0 x \hat{e}_y \) and \( \phi = -\varepsilon_0 x \) so that \( \nabla \times \vec{A} = -\varepsilon_0 \hat{e}_x \). We then have

\[
\hat{H} = \frac{1}{2m} \left( \hat{p}^2 - \frac{q}{c} \vec{A}(\vec{r}) \right)^2 + q\phi = \frac{1}{2m} \left( \hat{p}_x^2 + \left( \hat{p}_y - \frac{qB_0}{c} \right)^2 + \hat{p}_z^2 \right) - q\varepsilon_0 \hat{x}
\]

Since \( \hat{H} \) does not depend on \( \hat{y} \) and \( \hat{z} \) explicitly, we have

\[
\left[ \hat{H}, \hat{p}_y \right] = 0 = \left[ \hat{H}, \hat{p}_z \right]
\]

so that \( p_y \) and \( p_z \) are constants of the motion. That means we can replace operators by eigenvalues (numbers) to get

\[
\hat{H} = \frac{1}{2m} \hat{p}_x^2 + \frac{q^2 B_0^2}{2mc^2} \left( \hat{x} - cp_y \frac{qB_0}{EB_0} \right)^2 + \frac{1}{2m} \hat{p}_z^2 - \frac{mc^2 \varepsilon_0}{EB_0} - \frac{cp_y \varepsilon_0}{B_0}
\]

Now let

\[
\hat{\xi} = \hat{p}_x , \quad \hat{\xi} = \hat{x} - cp_y \frac{qB_0}{EB_0} , \quad \omega = \frac{|e| B_0}{mc}
\]

We then have

\[
\hat{H} = \frac{1}{2m} \hat{\xi}^2 + \frac{1}{2} m \omega^2 \hat{\xi}^2 + \frac{1}{2m} \hat{p}_z^2 - \frac{mc^2 \varepsilon_0^2}{2B_0^2} - \frac{cp_y \varepsilon_0}{B_0}
\]

Now,

\[
[\hat{x}, \hat{p}_x] = i\hbar \rightarrow \left[ \hat{\xi}, \hat{\xi} \right] = i\hbar \text{ (a new pair of conjugate variables)}
\]

This represents a simple harmonic oscillator. Therefore,

\[
E_n = (n + 1/2)\hbar \omega + \frac{1}{2m} \hat{p}_z^2 - \frac{mc^2 \varepsilon_0^2}{2B_0^2} - \frac{cp_y \varepsilon_0}{B_0} , \quad n = 0, 1, 2, \ldots
\]

(b) Find the expectation value of the velocity operator

\[
\bar{v} = \frac{1}{m} \hat{p}_\text{mechanical}
\]
in the state $\vec{p} = 0$.

A state of zero momentum signifies one in which $p_y = p_z = 0 = \langle \hat{p}_x \rangle$

Now we have
$$\vec{v} = \frac{1}{m} \vec{p}_{\text{mechanical}} = \frac{1}{m} \left( \vec{p} - \frac{q}{c} \vec{A} \right)$$

Therefore,
$$\langle \vec{v} \rangle = \frac{1}{m} \langle \vec{p} \rangle - \frac{q}{c} \langle \vec{A} \rangle = -\frac{q}{c} \langle \vec{A} \rangle = -\frac{qB_0}{mc} \langle \hat{x} \rangle \hat{e}_y$$

But,
$$\langle \hat{x} \rangle = \langle \hat{\xi} \rangle + \frac{c p_y}{q B_0} + \frac{mc^2 \varepsilon_0}{qB_0^2} = \frac{mc^2 \varepsilon_0}{qB_0^2}$$

Since
$$\langle \hat{\xi} \rangle = 0$$

Finally,
$$\langle \vec{v} \rangle = -\frac{qB_0}{mc} \langle \hat{x} \rangle \hat{e}_y = -\frac{c \varepsilon_0}{B_0} \hat{e}_y$$

### 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
$$ds^2 = c^2 dt^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2 - (dx^4)^2 - (dx^5)^2$$

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.

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 \(2\pi R\):

\[
P_1 \sim P_2 \leftrightarrow x(P_1) = x(P_2) + 2\pi Rn, \quad n \in \mathbb{Z} \quad (9.4)
\]

This is precise, but somewhat cumbersome, notation. With no risk of confusion, we can simply write

\[
x \sim x + 2\pi R \quad (9.5)
\]

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 see, 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.

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 $2\pi$ 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](image)

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 $\theta(P) = \text{angle}(POQ)$. This angle is naturally multi-valued. The reference point $Q$, for example, has $\theta(Q) = 0^\circ$ and $\theta(Q) = 360^\circ$. If we force angles to be
single-valued by restricting \(0^\circ \leq \theta \leq 360^\circ\), for example, then they become discontinuous. Indeed, two nearby points, \(Q\) and \(Q'\), then have very different angles \(\theta(Q) = 0^\circ\), while \(\theta(Q') \sim 360^\circ\). 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

\[
(x,y) \sim (x + 2\pi R, y) \quad , \quad (x,y) \sim (x,y + 2\pi R)
\]

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.
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.

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 the analysis of small extra dimensions, let us review the standard quantum mechanics problem involving an infinite potential well.

The time-independent Schrödinger 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 Schrödinger 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

\[
\psi_k(x) = \sqrt{\frac{2}{a}} \sin \left( \frac{k\pi x}{a} \right) , \quad k = 1, 2, \ldots, \infty
\]

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 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?

In two dimensions, the Schrodinger equation is given by

\[
-\frac{\hbar^2}{2m} \left( \frac{\partial^2 \psi(x, y)}{\partial x^2} + \frac{\partial^2 \psi(x, y)}{\partial y^2} \right) + V(x, y)\psi(x, y) = E\psi(x, y)
\]

Inside the well we have

\[
-\frac{\hbar^2}{2m} \left( \frac{\partial^2 \psi(x, y)}{\partial x^2} + \frac{\partial^2 \psi(x, y)}{\partial y^2} \right) = E\psi(x, y)
\]

We use separation of variables to solve this equation. We let

\[
\psi(x, y) = \alpha(x)\beta(y)
\]

and obtain

\[
-\frac{\hbar^2}{2m} \frac{1}{\alpha(x)} \left( \frac{d^2 \alpha(x)}{dx^2} \right) - \frac{\hbar^2}{2m} \frac{1}{\beta(y)} \left( \frac{d^2 \beta(y)}{dy^2} \right) = E
\]
The $x$–dependent and $y$–dependent terms of this equation must separately be constant. We obtain solution of the form

$$\psi_{kl}(x, y) = \alpha_k(x)\beta_l(y)$$

where

$$\alpha_k(x) = c_k \sin\left(\frac{k\pi x}{a}\right)$$

$$\beta_l(y) = a_l \sin\left(\frac{ly}{\pi}\right) + b_l \cos\left(\frac{ly}{\pi}\right)$$

The physics along the $x$ dimension is unchanged, since the wave-function must still vanish at the ends of the segment. Therefore, the solution $\alpha_k(x)$ takes the same form as earlier and $k = 1, 2, 3, \ldots$. The boundary condition for $\beta_l(y)$ arises from the identification $y \sim y + 2\pi R$. Since $y$ and $y + 2\pi R$ are coordinates that represent the same point, the wave-function must take the same value at these two arguments:

$$\beta_l(y) = \beta_l(y + 2\pi R)$$

The most general solution contains both sines and cosines in this case. The presence of the cosines allows a non-vanishing constant solution for $l = 0$ - we get $\beta_0(y) = b_0$. This solution is key to understanding why a small extra dimension does not change the low energy physics very much.

The energy eigenvalues of the $\psi_{kl}$ are

$$E_{kl} = \frac{\hbar^2}{2m} \left[ \left(\frac{k\pi}{a}\right)^2 + \left(\frac{l}{R}\right)^2 \right]$$

These energies correspond to doubly degenerate states when $l \neq 0$, because in this case the term

$$\beta_l(y) = a_l \sin\left(\frac{ly}{R}\right) + b_l \cos\left(\frac{ly}{R}\right)$$

contains two linearly independent solutions.

The extra dimension has changed the energy spectrum dramatically. We will see, however, that if $R << a$, then the low-lying part of the spectrum is unchanged. The rest of the spectrum changes, but these changes are not accessible in low energy experiments.

Since $l = 0$ is permitted, the energy levels $E_{k0}$ coincide with the old energy levels $E_k$! The new system contains all the energy levels of the old system. However, it also includes additional energy levels. What is the lowest new level? To minimize the energy, each of the terms in the result for $E_{kl}$ must be as low as possible. The minimum occurs when $k = 1$, since $k = 0$ is not allowed, and $l = 1$, since $l = 0$ gives us the old levels. The lowest new energy level is

$$E_{11} = \frac{\hbar^2}{2m} \left[ \left(\frac{\pi}{a}\right)^2 + \left(\frac{1}{R}\right)^2 \right]$$
When $R \ll a$, the second term is much larger than the first and thus

$$E_{11} \approx \frac{\hbar^2}{2m} \left( \frac{1}{R} \right)^2$$

This energy is comparable to that of the level $k$ eigenstate of the original problem where

$$\frac{k\pi}{a} \sim \frac{1}{R} \rightarrow k \sim \frac{1}{\pi R}$$

Since $R$ is much smaller than $a$, $k$ is a very large number. So the first new level appears at an energy far above that of the low-lying original states. We therefore conclude that an extra dimension can remain hidden from experiments at a particular energy level as long as the dimension is small enough. Once the probing energies become sufficiently high, the effect of an extra dimension can be observed.

The quantum mechanics of a string introduces new features not present here. For an extra dimension much smaller than the already small string length $\ell_s$, new low-lying states can appear! These correspond to the strings that wrap around the extra dimension. They have no analog in the quantum mechanics of a point particle. In string theory, the conclusion remains true that no new low energy states arise from a small extra dimension, but there is a small qualification - the dimension must not be significantly smaller than $\ell_s$.

9.7.40 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

$$H = A + B \mathbf{L} \cdot \mathbf{S} + C \mathbf{L} \cdot \mathbf{L}$$

What are the values of energy for each of the different states of total angular momentum in terms of the constants $A$, $B$, and $C$?

We have $\mathbf{J} = \mathbf{L} + \mathbf{S}$, $L = 2$, $S = 1/2$. Thus, the possible values for $j$ are 5/2 and 3/2 ($\ell + s \geq j \geq |\ell - s|$).

Now

$$H |j, m\rangle = (A + B \mathbf{L} \cdot \mathbf{S} + C \mathbf{L} \cdot \mathbf{L}) |j, m\rangle$$

where $|j, m\rangle = |\ell, s; j, m\rangle$.

Then, we have

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2} (J^2 - L^2 - S^2)$$
\[ \mathbf{L} \cdot \mathbf{S} |\ell, s; j, m\rangle = \frac{1}{2} (J^2 - L^2 - S^2) |\ell, s; j, m\rangle = \frac{1}{2} \hbar^2 (j(j+1) - \ell(\ell+1) - s(s+1)) |\ell, s; j, m\rangle = \frac{1}{2} \hbar^2 \left( j(j+1) - g - \frac{3}{4} \right) |\ell, s; j, m\rangle \]

\[ \mathbf{L} \cdot \mathbf{L} = L^2 \]

\[ \mathbf{L} \cdot \mathbf{L} = L^2 |\ell, s; j, m\rangle = \hbar^2 \ell(\ell+1) |\ell, s; j, m\rangle = 6\hbar^2 |\ell, s; j, m\rangle \]

so that

\[ H |j, m\rangle = (A + \frac{1}{2} B \hbar^2 \left( j(j+1) - g - \frac{3}{4} \right) + 6 Ch^2) |j, m\rangle = E_{jm} |j, m\rangle \]

Thus,

For \( j = \frac{5}{2} \) \( E_{jm} = A + B \hbar^2 + 6 Ch^2 \) independent of \( m \)

For \( j = \frac{3}{2} \) \( E_{jm} = A - \frac{3}{2} B \hbar^2 + 6 Ch^2 \) independent of \( m \)

### 9.7.41 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 \( S = (\hbar/2) \vec{\sigma} \cdot \hat{e} \), where \( \vec{\sigma} \) is represented by the Pauli matrices:

\[ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

Calculate the eigenvalues of \( \vec{S} \). The vector \( \vec{sigma} \) is defined as a vector whose components are matrices:

\[ \vec{\sigma} = \sigma_1 \hat{x} + \sigma_2 \hat{y} + \sigma_3 \hat{z} \]

Taking the dot product with the vector \( \hat{e} \) gives

\[ M = \frac{2}{\hbar} S = \sin \theta \sigma_1 + \cos \theta \sigma_2 \]

The matrix \( S \) represents the angular momentum along the vector \( \hat{e} \), so we expect that the eigenvalues must be \( \pm \hbar/2 \) or the matrix \( M \) must have eigenvalues \( \pm 1 \). To prove this, we solve \( M \psi = \lambda \psi \). As usual, this requires the zero determinant \( |N - \lambda I| = 0 \):

\[ \begin{vmatrix} \cos \theta - \lambda & \sin \theta \\ \sin \theta & -\cos \theta - \lambda \end{vmatrix} = \lambda^2 - \cos^2 \theta - \sin^2 \theta = \lambda^2 - 1 = 0 \]

Hence, the eigenvalues are as expected.
(b) Calculate the normalized eigenvectors of $\vec{S}$.

For the eigenvectors we need $M\psi = \pm \psi$. Writing $\psi$ as a 2-component vector

$$\psi = \begin{pmatrix} A \\ B \end{pmatrix}$$

we get the two equations

$$A \cos \theta + B \sin \theta = \pm A$$
$$A \sin \theta - B \cos \theta = \pm B$$

These give

$$\frac{A}{B} = \sin \theta (\pm 1 - \cos \theta)$$
$$\frac{A}{B} = \frac{\cos \theta \pm 1}{\sin \theta}$$

but these are the same equation (divide by the RHS), so we only get the ratio, which is reasonable since we have not used normalization yet (the second equation). Therefore,

$$\psi_{\pm} = N_{\pm} \left( \begin{pmatrix} \sin \theta \\ \pm 1 - \cos \theta \end{pmatrix} \right)$$

where $N$ is the normalization factor. We require the vector be normalized to 1 so that $|N|^2 = (2 \mp \cos \theta)^{-1}$.

(c) Calculate the intensities of the two beams which emerge from the second Stern-Gerlach apparatus.

Finally, we write

$$|\uparrow\rangle = \alpha \psi_+ + \beta \psi_-$$

where the coefficients $\alpha$ and $\beta$ come from the scalar product of $|\uparrow\rangle$ with $\psi_+$ and $\psi_-$, i.e.,

$$\alpha = \langle \uparrow | \uparrow \rangle = (1 \quad 0) N_+ \begin{pmatrix} \sin \theta \\ \pm 1 - \cos \theta \end{pmatrix} = N_+ \sin \theta$$

and

$$\beta = \langle \uparrow | \downarrow \rangle = (1 \quad 0) N_- \begin{pmatrix} \sin \theta \\ \pm -1 - \cos \theta \end{pmatrix} = N_- \sin \theta$$

The ratio of the two beam intensities is given by

$$\frac{|\alpha|^2}{|\beta|^2} = \frac{|N_+|^2}{|N_-|^2} = \frac{1 + \cos \theta}{1 - \cos \theta} = \cot^2 \left( \frac{\theta}{2} \right)$$

9.7.42 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.
Calculate the resulting intensity pattern recorded at the detector screen.

This calculation is the same for all particles independent of the spin value.

We assume that a spherical wave

\[ \psi(r, t) \sim \frac{e^{i(kr - \omega t)}}{r} \]

with momentum \( p = \hbar k \) extends from the source and one is generated at each slit. The probability amplitude at the detector screen then becomes the superposition of probability amplitudes of the waves from the three slits:

\[ \psi(x, t) \sim \frac{e^{i(kr_1 - \omega t)}}{r_1} + \frac{e^{i(kr_2 - \omega t)}}{r_2} + \frac{e^{i(kr_3 - \omega t)}}{r_3} \]

and the measured intensity at the detector screen is

\[ I \sim |\psi(x)|^2 \sim \left| \frac{e^{i(kr_1 - \omega t)}}{r_1} + \frac{e^{i(kr_2 - \omega t)}}{r_2} + \frac{e^{i(kr_3 - \omega t)}}{r_3} \right|^2 \]

and so on.

### 9.7.43 Cylindrical potential

The Hamiltonian is given by

\[ \hat{H} = \frac{\hat{p}^2}{2\mu} + V(\hat{\rho}) \]

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 $\hat{H}$.

Since the Hamiltonian is invariant under translations along the $z$–axis (the potential energy does not depend on $z$), the Hamiltonian must commute with $\hat{p}_z$, the generator of $z$–translations.

Similarly, since the Hamiltonian is invariant under rotations about the $z$–axis (the potential energy does not depend on the azimuthal angle $\phi$), the Hamiltonian must commute with $\hat{L}_z$, the generator of these rotations.

(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 $\hat{L}_z$.

Part (a) says that $|E, p_z, m\rangle$ is a simultaneous eigenstate of $\hat{H}$, $\hat{p}_z$, $\hat{L}_z$. We then have

$$\langle \vec{r} | E, p_z, m \rangle = \frac{e^{ip_z \rho / \hbar}}{\sqrt{2\pi \hbar}} \frac{e^{im\phi}}{\sqrt{2\pi R}} R(\rho)$$

(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 $\mu$ is in the cylindrical potential well

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

The energy eigenvalue equation in position space is

$$E_{n\alpha} = \frac{\hbar^2}{2\mu a^2} z_{n\alpha}^2 \quad , \quad z_{n\alpha} = n^{th} \text{ zero of } J_\alpha$$

$$\langle \vec{r} | \hat{H} | E, p_z, m \rangle = \left( -\frac{\hbar^2}{2\mu} \nabla^2 + V(\rho) \right) \langle \vec{r} | E, p_z, m \rangle = E \langle \vec{r} | E, p_z, m \rangle$$

Using the Laplacian in cylindrical coordinates

$$\nabla^2 \psi = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \varphi^2} + \frac{\partial^2 \psi}{\partial z^2}$$

we have

$$\left( -\frac{\hbar^2}{2\mu} \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial R}{\partial \rho} \right) + \frac{\hbar^2}{2\mu} \frac{\partial^2 R}{\partial \rho^2} + \frac{\hbar^2}{2\mu} \frac{\partial^2 R}{\partial \varphi^2} + \frac{\hbar^2}{2\mu} \frac{\partial^2 R}{\partial z^2} + V(\rho) \right) \frac{e^{ip_z \rho / \hbar}}{\sqrt{2\pi \hbar}} \frac{e^{im\phi}}{\sqrt{2\pi}} = E \frac{e^{ip_z \rho / \hbar}}{\sqrt{2\pi \hbar}} \frac{e^{im\phi}}{\sqrt{2\pi}} R$$

$$-\frac{\hbar^2}{2\mu} \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial R}{\partial \rho} \right) + \frac{\hbar^2}{2\mu} \frac{\partial^2 R}{\partial \rho^2} + \frac{\hbar^2}{2\mu} \frac{\partial^2 R}{\partial \varphi^2} + \frac{\hbar^2}{2\mu} \frac{\partial^2 R}{\partial z^2} + V(\rho) \right) R = ER$$

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Now rearranging and using 
\[ \lambda^2 = \frac{2\mu E}{\hbar^2}, \quad p_z = \hbar k \]
we have
\[ \rho^2 \frac{d^2 R}{d\rho^2} + \frac{dR}{d\rho} + \left(\lambda^2 \rho^2 - (m^2 + k^2)\right) R - \frac{2\mu}{\hbar^2} \rho^2 V(\rho) R = 0 \]

(d) Determine the three lowest energy eigenvalues for states that also have \( \hat{p}_z \) and \( \hat{L}_z \) equal to zero.

For
\[ V(\rho) = \begin{cases} 0 & \rho < a \\ \infty & \rho > a \end{cases} \]
we have for \( \rho < a \)
\[ \rho^2 \frac{d^2 R}{d\rho^2} + \frac{dR}{d\rho} + \left(\lambda^2 \rho^2 - (m^2 + k^2)\right) R = 0 \quad \text{and} \quad R(a) = 0 \]
which is Bessel’s equation. Letting \( \alpha^2 = m^2 + k^2 \) we have
\[ R(\rho) = AJ_\alpha(\lambda\rho) \]
We have excluded the Bessel functions of the 2nd kind since they are not finite at \( \rho = 0 \).

The boundary condition becomes \( J_\alpha(\lambda a) = 0 \) so that \( \lambda a = n \) zero of \( J_\alpha \).

Therefore,
\[ E_{n\alpha} = \frac{\hbar^2}{2\mu a^2} \lambda^2 a^2, \quad z_{n\alpha} = n^{th} \text{ zero of } J_\alpha \]

When \( p_z = \hbar k = 0 = m \rightarrow \alpha = 0 \) we are looking for the zeroes of \( J_0 \). The three lowest energy eigenvalues are then
\[ E_1 = \frac{\hbar^2}{2\mu a^2} (2.4048)^2 \]
\[ E_2 = \frac{\hbar^2}{2\mu a^2} (5.5201)^2 \]
\[ E_3 = \frac{\hbar^2}{2\mu a^2} (8.6537)^2 \]

(e) Determine the three lowest energy eigenvalues for states that also have \( \hat{p}_z \) equal to zero. The states can have nonzero \( \hat{L}_z \).

For \( p_z = \hbar k = 0 \), we have
\[ J_0(z) = 0 \rightarrow z = 2.40, 5.52, 8.65 \]
\[ J_1(z) = 0 \rightarrow z = 3.83, 7.02, 10.17 \]
\[ J_2(z) = 0 \rightarrow z = 5.14, 8.42, 11.62 \]
and therefore the three lowest energies are

\[ E_1 = \frac{\hbar^2}{2m_a^2} (2.4048)^2 \quad p_z = 0, m = 0 \rightarrow 1^{st} \text{ zero of } J_0 \]

\[ E_2 = \frac{\hbar^2}{2m_a^2} (3.8317)^2 \quad p_z = 0, m = 1 \rightarrow 1^{st} \text{ zero of } J_1 \]

\[ E_3 = \frac{\hbar^2}{2m_a^2} (5.1356)^2 \quad p_z = 0, m = 2 \rightarrow 1^{st} \text{ zero of } J_2 \]

### 9.7.44 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 \( A > 0, B > 0, |\lambda| < 1 \). \( \mu \) is arbitrary. Find the energy eigenvalues.

We choose two new variables

\[
\begin{align*}
  u &= \frac{1}{\sqrt{2}} (x + y) \quad , \quad t = \frac{1}{\sqrt{2}} (x - y) \\
  x &= \frac{u + t}{\sqrt{2}} \quad , \quad y = \frac{u - t}{\sqrt{2}}
\end{align*}
\]

The potential energy becomes

\[
V(x, y, z) = A \left( \left( \frac{u + t}{\sqrt{2}} \right)^2 + \left( \frac{u - t}{\sqrt{2}} \right)^2 + 2\lambda \left( \frac{u + t}{\sqrt{2}} \right) \left( \frac{u - t}{\sqrt{2}} \right) \right) + B \left( z^2 + 2\mu z \right)
\]

\[ = A \left[ (1 + \lambda) u^2 + (1 - \lambda) t^2 \right] + B \left( z^2 + 2\mu z \right)\]

The derivatives become

\[
\begin{align*}
  \frac{\partial}{\partial x} &= \frac{1}{\sqrt{2}} \frac{\partial}{\partial u} + \frac{1}{\sqrt{2}} \frac{\partial}{\partial t} \\
  \rightarrow \frac{\partial^2}{\partial x^2} &= \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} \frac{\partial^2}{\partial u^2} + \frac{1}{\sqrt{2}} \frac{\partial^2}{\partial u \partial t} \right) + \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} \frac{\partial^2}{\partial t^2} + \frac{1}{\sqrt{2}} \frac{\partial^2}{\partial u \partial t} \right)
\end{align*}
\]

\[
\begin{align*}
  \frac{\partial}{\partial y} &= \frac{1}{\sqrt{2}} \frac{\partial}{\partial u} - \frac{1}{\sqrt{2}} \frac{\partial}{\partial t} \\
  \rightarrow \frac{\partial^2}{\partial y^2} &= \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} \frac{\partial^2}{\partial u^2} - \frac{1}{\sqrt{2}} \frac{\partial^2}{\partial u \partial t} \right) - \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} \frac{\partial^2}{\partial t^2} + \frac{1}{\sqrt{2}} \frac{\partial^2}{\partial u \partial t} \right)
\end{align*}
\]

so that

\[ \nabla^2 = \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial z^2} \]

and the Schrödinger equation becomes

\[
\left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial z^2} \right) \varphi(u, t, z) + \frac{2m}{\hbar^2} (E - V(u, t, z)) \varphi(u, t, z) = 0
\]
We now separate variables. Substituting \( \varphi(u, t, z) = U(u)T(t)Z(z) \) gives

\[
\begin{align*}
\frac{\partial^2 U}{\partial u^2} + \frac{2m}{\hbar^2} (E_1 + A(1 + \lambda)u^2) U &= 0 \\
\frac{\partial^2 T}{\partial t^2} + \frac{2m}{\hbar^2} (E_2 - A(1 - \lambda)t^2) T &= 0 \\
\frac{\partial^2 Z}{\partial z^2} + \frac{2m}{\hbar^2} (E_3 - B(z^2 + 2\mu z)) Z &= 0
\end{align*}
\]

where the separation constants are chosen so that \( E = E_1 + E_2 + E_3 \).

If we set \( z' = z + \mu \) and \( E_3' = E_3 + \mu^2 \) all of the above equations reduce to harmonic oscillators. Therefore,

\[
\begin{align*}
E_1 &= (n_1 + 1/2)\hbar \omega_1, \quad \omega_1 = \sqrt{\frac{2A}{m}(1 + \lambda)} \\
E_2 &= (n_2 + 1/2)\hbar \omega_2, \quad \omega_2 = \sqrt{\frac{2A}{m}(1 - \lambda)} \\
E_3 &= (n_3 + 1/2)\hbar \omega_3 - B\mu^2, \quad \omega_3 = \sqrt{\frac{2m}{B}}
\end{align*}
\]

where \( n_1, n_2, n_3 = 0, 1, 2, 3, \ldots \).

(b) Now consider the following modified problem with a new potential

\[
V_{\text{new}} = \begin{cases} 
V(x, y, z) & z > -\mu \text{ and any } x \text{ and } y \\
+\infty & z < -\mu \text{ and any } x \text{ and } y
\end{cases}
\]

Find the ground state energy.

The wave function must now vanish for \( z = -\mu \).

This has no effect on the \( U(u) \) and \( T(t) \) solutions.

The original \( Z(z) \) equation had the solutions

\[
Z(z) = H_{n_3}(\zeta)e^{-\zeta^2}, \quad \zeta = \left( \frac{2mB}{\hbar^2} \right)^{1/4}(z + \mu)
\]

where \( H_{n_3} \) are the Hermite polynomials.

We need solutions that are zero at \( \zeta = 0 \) or \( z = -\mu \). These are the odd parity solutions where the parity of the solutions is given by \((-1)^{n_3} \) so that the only allowed solutions now correspond to \( n_3 = 1, 3, 5, \ldots \).

The old ground state was \( n_1 = n_2 = n_3 = 0 \). The new ground state is \( n_1 = n_2 = 0, n_3 = 1 \).

The old ground state energy was

\[
E_0 = \frac{1}{2}\hbar(\omega_1 + \omega_2 + \omega_3) - B\mu^2
\]

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The new ground state energy is

\[ E'_0 = \frac{1}{2} \hbar (\omega_1 + \omega_2 + 3\omega_3) - B\mu^2 \]

9.7.45 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 \( \theta \) 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?

As preparation we determine the eigenvectors corresponding to the eigenvalues \( m_y \hbar, \ m_y = 1, 0, -1 \) of \( S_y \). From \( S_y |m_y\rangle = m_y \hbar |m_y\rangle \) we obtain (using problem 9.7.15)

\[
\frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = m_y \hbar \begin{pmatrix} a \\ b \\ c \end{pmatrix}
\]

or

\[
-ib = m_y a \\
-b = i\sqrt{2} a - i\frac{\hbar}{\sqrt{2}} c = m_y b \\
i\sqrt{2} b = m_y c
\]

These give

\[
|m_y = \pm 1\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ \pm \sqrt{2} i \\ -1 \end{pmatrix}, \quad |m_y = 0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
\]

Now we can solve the problem. The incoming state into the second device is

\[
|m_z = 1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
\]

The second device is rotated by \( \theta \) around the \( y \)-axis. The outcome of the experiment can be calculated in many ways. Here we consider rotating the state by \( -\theta \) around the \( y \)-axis and sending it through an unrotated \( SG_z \) device. The incident state thus becomes:

\[
|\psi\rangle = R_y(-\theta) |m_z = 1\rangle = e^{-iS_y(-\theta)/\hbar} |m_z = 1\rangle
\]

We evaluate this by the completeness relation of eigenstates of \( S_y \):

\[
|\psi\rangle = \sum_{m_y} e^{iS_y \theta / \hbar} |m_y\rangle \langle m_y | m_z = 1\rangle
\]

\[
= e^{i\theta} |m_y = 1\rangle \langle m_y = 1 | m_z = 1\rangle + |m_y = 0\rangle \langle m_y = 0 | m_z = 1\rangle
\]

\[
+ e^{-i\theta} |m_y = -1\rangle \langle m_y = -1 | m_z = 1\rangle
\]

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The amplitude of the spin-up state exiting the second device is
\[ \langle m_z = 1 | \psi \rangle = e^{i\theta} | \langle m_y = 1 | m_z = 1 \rangle |^2 + | \langle m_y = 0 | m_z = 1 \rangle |^2 \]
\[ = \frac{e^{i\theta}}{4} + \frac{1}{2} + \frac{-e^{i\theta}}{4} = \frac{1 + \cos \theta}{2} \]
The fraction of particles exiting is the probability
\[ N_{+1}(\theta) = | \langle m_z = 1 | \psi \rangle |^2 = \frac{(1 + \cos \theta)^2}{4} \]
Note that \( N(\theta = 0) = 1 \) and \( N(\theta = \pi) = 0 \) as expected. One can check by the same method to obtain
\[ N_{-1}(\theta) = \frac{(1 - \cos \theta)^2}{4} = N_{+1}(\pi - \theta), \quad N_0(\theta) = \frac{\sin^2 \theta}{2} \]
so that \( N_{+1} + N_{-1} + N_0 = 1 \).

**9.7.46 Three Spherical Harmonics**

As we see, often we need to calculate an integral of the form
\[ \int d\Omega Y^{\ast}_{\ell_3 m_3}(\theta, \varphi) Y_{\ell_2 m_2}(\theta, \varphi) Y_{\ell_1 m_1}(\theta, \varphi) \]
This can be interpreted as the matrix element \( \langle \ell_3 m_3 | \hat{Y}^{(\ell_2)} | \ell_1 m_1 \rangle \), where \( \hat{Y}^{(\ell_2)} \) 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.

We have
\[ \langle \ell_3 m_3 | \hat{Y}^{(\ell_2)} | \ell_1 m_1 \rangle = \int d\Omega Y^{\ast}_{\ell_3 m_3}(\theta, \varphi) Y_{\ell_2 m_2}(\theta, \varphi) Y_{\ell_1 m_1}(\theta, \varphi) \]
\[ = \langle \ell_3 || \hat{Y}^{(\ell_2)} || \ell_1 \rangle \langle \ell_3 m_3 | \ell_2 m_2 \ell_1 m_1 \rangle \]
where we have used the Wigner-Eckart theorem.

Thus, this integral vanishes unless
\[ m_3 = m_2 + m_1 \]
\[ |\ell_2 - \ell_1| \leq \ell_3 \leq \ell_2 + \ell_1 \]

(b) Given the addition rule for Legendre polynomials:
\[ P_{\ell_2}(\mu)P_{\ell_3}(\mu) = \sum_{\ell_4} \langle \ell_4 0 | \ell_1 0 \ell_2 0 \rangle^2 P_{\ell_4}(\mu) \]

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Therefore, now
\[ P_\ell (\cos \theta) = \sqrt{\frac{2\ell + 1}{4\pi}} P_\ell (\cos \theta) \]
where \( P_\ell (\cos \theta) \) is the Legendre polynomial. This implies that
\[ \langle \ell_3 | \hat{Y}_0^{(\ell_2)} | \ell_1 \rangle \]
Now
\[ P_{\ell_1} (\cos \theta) P_{\ell_2} (\cos \theta) = \sum_{\ell'} \langle \ell' | \ell_1, \ell_2 \rangle^2 P_{\ell'} (\cos \theta) \]
Therefore,
\[ \int d\Omega Y_{\ell_3 m_3}^* (\theta, \varphi) Y_{\ell_2 m_2} (\theta, \varphi) Y_{\ell_1 m_1} (\theta, \varphi) \]
\[ = \sqrt{\frac{(2\ell_2 + 1)(2\ell_1 + 1)}{4\pi(2\ell_3 + 1)}} \langle \ell_3, \ell_1, \ell_2 \rangle \]
This implies that we can solve for the reduced matrix element. Putting it all together, we have
\[ \int d\Omega Y_{\ell_3 m_3}^* (\theta, \varphi) Y_{\ell_2 m_2} (\theta, \varphi) Y_{\ell_1 m_1} (\theta, \varphi) \]
\[ = \sqrt{\frac{(2\ell_2 + 1)(2\ell_1 + 1)}{4\pi(2\ell_3 + 1)}} \langle \ell_3, \ell_1, \ell_2 \rangle \]
\[ \langle \ell_3 | \hat{Y}_0^{(\ell_2)} | \ell_1 \rangle \]

\[ \langle \ell_3 | \hat{Y}_0^{(\ell_2)} | \ell_1 \rangle \]
9.7.47 Spin operators ala Dirac

Show that

\[ \hat{S}_z = \frac{\hbar}{2} |z+\rangle \langle z+| - \frac{\hbar}{2} |z-\rangle \langle z-| \]
\[ \hat{S}_+ = \hbar |z+\rangle \langle z-| \]
\[ \hat{S}_- = \hbar |z-\rangle \langle z+| \]

We have the general spectral decomposition of an operator

\[ \hat{Q} = \sum_k Q_k |Q_k\rangle \langle Q_k| \]
\[ \hat{Q} |Q_k\rangle = Q_k |Q_k\rangle \]

Therefore,

\[ \hat{S}_z = \frac{\hbar}{2} |+z\rangle \langle +z| - \frac{\hbar}{2} |-z\rangle \langle -z| \]

Now

\[ |\pm x\rangle = \frac{1}{\sqrt{2}} |+z\rangle \pm \frac{1}{\sqrt{2}} |-z\rangle \]

so that

\[ \hat{S}_x = \frac{\hbar}{2} |x\rangle \langle x| - \frac{\hbar}{2} |-x\rangle \langle -x| \]

\[ = \frac{\hbar}{2} \left( \frac{1}{2} (|+z| + |-z|) (|+z\rangle + |-z\rangle) - \frac{1}{2} (|+z| - |-z|) (|+z\rangle - |-z\rangle) \right) \]
\[ = \frac{\hbar}{2} |+z\rangle \langle -z| + \frac{\hbar}{2} |-z\rangle \langle +z| \]

and since

\[ |\pm y\rangle = \frac{1}{\sqrt{2}} |+z\rangle \pm \frac{i}{\sqrt{2}} |-z\rangle \]

we get in a similar manner

\[ \hat{S}_x = \frac{\hbar}{2} |y\rangle \langle y| - \frac{\hbar}{2} |-y\rangle \langle -y| = -\frac{i\hbar}{2} |+z\rangle \langle -z| + \frac{i\hbar}{2} |-z\rangle \langle +z| \]

Then

\[ \hat{S}_\pm = \frac{\hat{S}_x \pm i\hat{S}_y}{2} = \hbar |\mp z\rangle \langle \mp z| \]

Some other checks: we find

\[ \hat{S}_z |\pm z\rangle = \pm \frac{\hbar}{2} |\pm z\rangle \]
\[ \hat{S}_+ |+z\rangle = 0 \]
\[ \hat{S}_- |+z\rangle = \hbar |-z\rangle \]
\[ \hat{S}_+ |-z\rangle = \hbar |+z\rangle \]
\[ \hat{S}_- |-z\rangle = 0 \]

which are all consistent with the general relations

\[ \hat{S}_z |s, m\rangle = m\hbar |s, m\rangle \]
\[ \hat{S}_\pm |s, m\rangle = \sqrt{s(s+1 - m(m \pm 1))}\hbar |s, m \pm 1\rangle \]

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9.7.48 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 $0 \leq a \leq 1$. What is the most general possibility for the state?

We consider first the case of a pure state

$$|\psi\rangle = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + z \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = x |1, 1\rangle + y |1, 0\rangle + z |1, -1\rangle$$

where $|1, m\rangle$ is the normalized eigenvector of $\hat{S}_3$ belonging to the eigenvalue $m$ (assuming $\hbar = 1$). Since the matrix elements of $\hat{S}_1$ and $\hat{S}_2$ vanish, so do the matrix elements of $\hat{S}_\pm = \hat{S}_1 \pm i \hat{S}_2$, and since

$$\hat{S}_+ |1, 1\rangle = 0 \quad \hat{S}_+ |1, 0\rangle = \sqrt{2} |1, 1\rangle \quad \hat{S}_+ |1, -1\rangle = \sqrt{2} |1, 0\rangle$$

it follows that

$$\langle \psi | \hat{S}_+ |\psi\rangle = \sqrt{2} (x^* y + y^* z) \to x^* y = -y^* z$$

We also have

$$\langle \psi | \hat{S}_2 |\psi\rangle = (x^* x - z^* z) = a = |x|^2 - |z|^2$$

and normalization gives

$$|x|^2 + |y|^2 + |z|^2 = 1$$

These equations imply that

$$|x||y| = |z||y| \to \left(|x|^2 - |z|^2\right)|y|^2 = 0$$

Combining these equations we have $a |y|^2 = 0$.

**Case #1:** If $a \neq 0$, then necessarily $|y|^2 = 0$. Then

$$|x|^2 - |z|^2 = a \quad |x|^2 + |z|^2 = 1$$

$$|x|^2 = \frac{1+a}{2} \quad |z|^2 = \frac{1-a}{2}$$

Since overall phase is not important we then have

$$|\psi\rangle = \begin{pmatrix} \sqrt{\frac{1+a}{2}} \\ 0 \\ \sqrt{\frac{1-a}{2}} e^{i\varphi} \end{pmatrix}$$

with just one free parameter, the relative phase $\varphi$. In the special subcase $a = 1$, this reduces to the unique solution $|1, 1\rangle$. 

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Case #2: The case \( a = 0 \) requires special treatment. Now \(|y|\) need not vanish, and we find that, in general,
\[
\left( |x|^2 - |z|^2 \right) |y|^2 = 0 \rightarrow |x| = |z| = \alpha
\]
If we fix the overall phase by requiring that \( y \) be real, then we have
\[
x^* y = -y^* z = -yz \rightarrow x^* = -z
\]
Now, the normalization condition gives
\[
|x|^2 + |y|^2 + |z|^2 = 1 = 2\alpha^2 + y^2 \rightarrow y = \sqrt{1 - 2\alpha^2}
\]
The general solution is then
\[
|\psi\rangle = \begin{pmatrix}
\alpha e^{i\varphi} \\
\sqrt{1 - 2\alpha^2} \\
-\alpha e^{-i\varphi}
\end{pmatrix}
\]
which depends on two parameters, \( \alpha \) and \( \varphi \).

The above discussion applies to pure states.

More generally, a state can be expressed by an operator of the form
\[
\hat{\rho} = \sum_{i=-1}^{1} \sum_{j=-1}^{1} \rho_{ij} |1, i\rangle \langle 1, j|
\]
where \( \rho_{ij} = \rho_{ji}^* \) since the operator is Hermitian. Therefore, there are three real diagonal elements, but only two are independent because of the normalization condition \( Tr\hat{\rho} = 1 \). There are three complex elements above the diagonal which corresponds to six real numbers that determine the non-diagonal elements above and below the diagonal. The conditions and yield three real constraints on these eight numbers, thus leaving five real parameters for the general solution, say \( c_1, c_2, c_3, c_4, c_5 \) as shown below.

\[
\hat{\rho} = \begin{pmatrix}
c_1 & c_2 + ic_3 & c_4 + ic_5 \\
c_2 - ic_3 & 1 + a - 2c_1 & -c_2 - ic_3 \\
c_4 - ic_5 & -c_2 + ic_3 & c_1 - a
\end{pmatrix}
\]

Clearly, there is much more freedom for a general state than for a pure state.

9.7.49 Properties of an operator

An operator \( \hat{f} \) describing the interaction of two spin\(-1/2\) particles has the form
\[
\hat{f} = a + b\hat{\sigma}_1 \cdot \hat{\sigma}_2 \quad \text{where} \quad a \quad \text{and} \quad b \quad \text{are constants and} \quad \hat{\sigma}_j = \sigma_{xj} \hat{x} + \sigma_{yj} \hat{y} + \sigma_{zj} \hat{z} \quad \text{are Pauli matrix operators.} \quad \text{The total spin angular momentum is}
\]
\[
\hat{j} = \hat{j}_1 + \hat{j}_2 = \frac{\hbar}{2} (\hat{\sigma}_1 + \hat{\sigma}_2)
\]
(a) Show that \( \hat{f}, \hat{J}^2 \) and \( \hat{J}_z \) can be simultaneously measured.

\( \hat{f}, \hat{J}^2, \hat{J}_z \) can be measured simultaneously if they all commute. Now we know that

\[
[\hat{J}_z, \hat{J}_z] = 0 = [\hat{J}^2, a] = [\hat{J}_z, a]
\]

Now

\[
\hat{J}^2 = \frac{\hbar^2}{4} (\hat{\sigma}_1 + \hat{\sigma}_2)^2 = \frac{\hbar^2}{4} (\hat{\sigma}_1^2 + \hat{\sigma}_2^2 + 2\hat{\sigma}_1 \cdot \hat{\sigma}_2) \rightarrow \hat{\sigma}_1 \cdot \hat{\sigma}_2 = \frac{2}{\hbar^2} \hat{J}^2 - \frac{1}{2} (\hat{\sigma}_1^2 + \hat{\sigma}_2^2)
\]

and

\[
\hat{\sigma}_1^2 = \hat{\sigma}_2^2 = 3 \rightarrow \hat{\sigma}_1 \cdot \hat{\sigma}_2 = \frac{2}{\hbar^2} \hat{J}^2 - 3
\]

Therefore,

\[
[\hat{J}_z, \hat{f}] = [\hat{J}_z, a] + b [\hat{J}_z, \hat{\sigma}_1 \cdot \hat{\sigma}_2] = b [\hat{J}_z, \frac{2}{\hbar^2} \hat{J}^2 - 3] = 0
\]

and

\[
[\hat{J}_z, \hat{J}^2] = [\hat{J}_z, a] + b [\hat{J}_z, \hat{J}_z \cdot \hat{\sigma}_2] = b [\hat{J}_z, \frac{2}{\hbar^2} \hat{J}^2 - 3] = 0
\]

so that \( \hat{f}, \hat{J}^2, \hat{J}_z \) can be measured simultaneously.

(b) Derive the matrix representation of \( \hat{f} \) in the \(|j, m, j_1, j_2\rangle \) basis.

In the \(|J, M, j_1, j_2\rangle \) basis we have

\[
(J, M, j_1, j_2 \langle \hat{f} | J', M', j_1, j_2 \rangle = a \delta_{JJ'} \delta_{MM'} + b (J, M, j_1, j_2 \langle J', M', j_1, j_2 \rangle \left( \frac{2}{\hbar^2} \hat{J}^2 - 3 \right) |J', M', j_1, j_2 \rangle
\]

\[
= (a + (2J(J + 1) - 3)b) \delta_{JJ'} \delta_{MM'}
\]

Since for two spin = 1/2 particles we have

\[
\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1
\]

The allowed \( J \) values are 0, 1 and the allowed states of the two-particle system are (letting \(|J, M, j_1, j_2\rangle \rightarrow |J, M\rangle\))

\[
|0, 0 \rangle, |1, 1 \rangle, |1, 0 \rangle, |1, -1 \rangle
\]

which give a diagonal matrix

\[
\hat{f} = \begin{pmatrix}
    a - 3b & 0 & 0 & 0 \\
    0 & a + b & 0 & 0 \\
    0 & 0 & a + b & 0 \\
    0 & 0 & 0 & a + b
\end{pmatrix}
\]

(c) Derive the matrix representation of \( \hat{f} \) in the \(|j_1, j_2, m_1, m_2\rangle \) basis.
We now use the basis (letting $|j_1, j_2, m_1, m_2\rangle \rightarrow |m_1, m_2\rangle$) since $j_1$ and $j_2$
do not change. We then write

$$\hat{f} = a + b\hat{\sigma}_1 \cdot \hat{\sigma}_2 = a + b(\hat{\sigma}_{1x}\hat{\sigma}_{2x} + \hat{\sigma}_{1y}\hat{\sigma}_{2y} + \hat{\sigma}_{1z}\hat{\sigma}_{2z})$$

$$= a + b\left(\frac{\hat{\sigma}_{1+} + \hat{\sigma}_{1-} - \hat{\sigma}_{2+} + \hat{\sigma}_{2-}}{2} + \frac{\hat{\sigma}_{1+} - \hat{\sigma}_{1-} + \hat{\sigma}_{2+} - \hat{\sigma}_{2-}}{2}\right)$$

$$= a + b\left(\frac{\hat{\sigma}_{1z}\hat{\sigma}_{2z}}{2} + \hat{\sigma}_{1z}\hat{\sigma}_{2z}\right)$$

The basis states are

$$|\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle, |\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle$$

and using

$$\hat{\sigma}_+|\frac{1}{2}\rangle = 0 = \hat{\sigma}_-|\frac{1}{2}\rangle, \quad \hat{\sigma}_+|\frac{1}{2}\rangle = 2|\frac{1}{2}\rangle, \quad \hat{\sigma}_-|\frac{1}{2}\rangle = 2|\frac{1}{2}\rangle$$

we have

$$\hat{f}|\frac{1}{2}, \frac{1}{2}\rangle = (a + 2b)|\frac{1}{2}, \frac{1}{2}\rangle$$

$$\hat{f}|\frac{1}{2}, -\frac{1}{2}\rangle = a|\frac{1}{2}, -\frac{1}{2}\rangle + b\left(4|\frac{1}{2}, \frac{1}{2}\rangle - |\frac{1}{2}, -\frac{1}{2}\rangle\right)$$

$$\hat{f}|\frac{1}{2}, \frac{1}{2}\rangle = a|\frac{1}{2}, \frac{1}{2}\rangle + b\left(4|\frac{1}{2}, -\frac{1}{2}\rangle - |\frac{1}{2}, \frac{1}{2}\rangle\right)$$

Then

$$\langle \frac{1}{2}, \frac{1}{2} | \hat{f} | \frac{1}{2}, \frac{1}{2}\rangle = (a + 2b)\langle \frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2}\rangle = (a + 2b)$$

$$\langle \frac{1}{2}, -\frac{1}{2} | \hat{f} | \frac{1}{2}, \frac{1}{2}\rangle = a\langle \frac{1}{2}, -\frac{1}{2} | \frac{1}{2}, -\frac{1}{2}\rangle + b\left(4\langle \frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2}\rangle - \langle \frac{1}{2}, -\frac{1}{2} | \frac{1}{2}, -\frac{1}{2}\rangle\right) = a - b$$

$$\langle \frac{1}{2}, -\frac{1}{2} | \hat{f} | \frac{1}{2}, -\frac{1}{2}\rangle = a\langle \frac{1}{2}, -\frac{1}{2} | \frac{1}{2}, -\frac{1}{2}\rangle + b\left(4\langle \frac{1}{2}, -\frac{1}{2} | \frac{1}{2}, -\frac{1}{2}\rangle - \langle \frac{1}{2}, -\frac{1}{2} | \frac{1}{2}, -\frac{1}{2}\rangle\right) = 4b$$

$$\langle \frac{1}{2}, -\frac{1}{2} | \hat{f} | \frac{1}{2}, -\frac{1}{2}\rangle = (a + 2b)\langle \frac{1}{2}, -\frac{1}{2} | \frac{1}{2}, -\frac{1}{2}\rangle = 0$$

so that

$$f = \begin{pmatrix}
    a + 2b & 0 & 0 & 0 \\
    0 & a - b & 4b & 0 \\
    0 & 4b & a - b & 0 \\
    0 & 0 & 0 & a + 2b
  \end{pmatrix}$$

9.7.50 Simple Tensor Operators/Operations

Given the tensor operator form of the particle coordinate operators

$$\vec{r} = (x, y, z); \quad R_0^1 = z, \quad R_1^1 = \mp \frac{x \pm iy}{\sqrt{2}}$$

(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

\[
[R^q_1, P^m_1] = \text{simple expression}
\]

We have

\[
R^\pm_1 = \mp \frac{R_x \pm iR_y}{\sqrt{2}}, \quad P^\pm_1 = \mp \frac{P_x \pm iP_y}{\sqrt{2}}
\]

We can write (for generality)

\[
R^q_1 = -q \frac{R_x \pm qiR_y}{\sqrt{2}}, \text{ etc}
\]

Now

\[
[R^q_1, P^m_1] = \frac{1}{2}q[mR_x \pm qiR_y, P_x \pm mP_y]
\]

\[
= \frac{1}{2}qm \left([R_x, P_x] + i^2qm[R_y, P_y]\right) = \frac{1}{2}qm(i\hbar) - \frac{1}{2}q^2m^2(i\hbar)
\]

\[
= \frac{i\hbar}{2}[qm - 1] = \begin{cases} -i\hbar & q \neq m \\ 0 & q = m \end{cases}
\]

So,

\[
[R^q_1, P^m_1] = -i\hbar(1 - \delta_{qm}) = -i\hbar\delta_{q,-m}
\]

Now,

\[
[R^0_1, P^0_1] = [Z, P_z] = i\hbar
\]

Clearly, \(R^0_1\) commutes with \(P^\pm_1\) and vice-versa.

A simple way to combine all of these results is

\[
[R^q_1, P^m_1] = (-1)^q i\hbar\delta_{q,-m}
\]

### 9.7.51 Rotations and Tensor Operators

Using the rank 1 tensor coordinate operator in Problem 9.7.50, calculate the commutators

\[
[L_\pm, R^q_1] \text{ and } [L_z, R^q_1]
\]

where \(\vec{L}\) is the standard angular momentum operator.
We have

\[
[L_z, R_1^q] = \left[ L_z, -q \frac{R_x + iqR_y}{\sqrt{2}} \right]
\]

\[
= -q \frac{1}{\sqrt{2}} [L_z, R_x] - i q^2 \frac{1}{\sqrt{2}} [L_z, R_y]
\]

\[
= -q \frac{i}{\sqrt{2}} (iR_y) - i \frac{q}{\sqrt{2}} (-iR_x)
\]

\[
= -q \frac{\hbar}{\sqrt{2}} (R_x + iqR_y)
\]

\[
= q \hbar R_1^q
\]

for \( q = \pm 1 \) (note that we used \( q^2 = 1 \) in the derivation). Note also that if \( q = 0 \), the commutator vanishes and this expression still works!

Now

\[
[L_x, R_1^q] = [L_x \pm iL_y, R_1^q]
\]

\[
= [L_x, R_1^q] \pm i[L_y, R_1^q]
\]

\[
= \left[ L_x, \frac{R_x + iqR_y}{\sqrt{2}} \right] \pm i \left[ L_y, \frac{R_x + iqR_y}{\sqrt{2}} \right]
\]

\[
= -q \frac{1}{\sqrt{2}} [L_x, R_x] - i \frac{q}{\sqrt{2}} [L_x, R_y] \pm i \left( -q \frac{1}{\sqrt{2}} [L_y, R_x] - i \frac{q}{\sqrt{2}} [L_y, R_y] \right)
\]

\[
= 0 - i \frac{q}{\sqrt{2}} (-z \hbar) \pm i \left( 0 - i \frac{q}{\sqrt{2}} (-z \hbar) \right)
\]

\[
= -z \hbar \frac{1}{\sqrt{2}} \pm i \left( z \hbar \frac{1}{\sqrt{2}} \right)
\]

\[
= -z \hbar \frac{1}{\sqrt{2}} R_1^0 (1 \pm 1)
\]

So it should be \( \pm \sqrt{2} \hbar R_1^0 \), if it is nonzero. It means

\[
[L_+, R_1^q = 0 = [L_-, R_1^{-1}] \quad [L_\pm, R_1^\mp] = \pm \sqrt{2} \hbar R_1^0.
\]

### 9.7.52 Spin Projection Operators

Show that \( \mathcal{P}_1 = \frac{3}{4} I + (\vec{S}_1 \cdot \vec{S}_2)/\hbar^2 \) and \( \mathcal{P}_0 = \frac{1}{4} I - (\vec{S}_1 \cdot \vec{S}_2)/\hbar^2 \) 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.

We have

\[
\vec{S}^2 = (\vec{S}_1 + \vec{S}_2)^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2 \vec{S}_1 \cdot \vec{S}_2
\]

We can easily answer this question in the \( \{S, M\} \) representation. We have

\[
\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2} \left( \vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2 \right)
\]

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\[ \vec{S}_1 \cdot \vec{S}_2 = \hbar^2 S_1 (S_1 + 1) = \frac{3\hbar^2}{4} \]

\[ \vec{S}_2 \cdot \vec{S}_2 = \hbar^2 S_2 (S_2 + 1) = \frac{3\hbar^2}{4} \]

Therefore,

\[ P_1 = \frac{3}{4} \hat{I} + (\vec{S}_1 \cdot \vec{S}_2) / \hbar^2 = \left( \frac{3}{4} + \frac{1}{2} S(S+1) - \frac{3}{4} \right) \hat{I} = \frac{1}{2} S(S+1) \hat{I} \]

\[ P_0 = \frac{1}{4} \hat{I} - (\vec{S}_1 \cdot \vec{S}_2) / \hbar^2 = \left( \frac{3}{4} + \frac{1}{2} S(S+1) - \frac{3}{4} \right) \hat{I} = \left( 1 - \frac{1}{2} S(S+1) \right) \hat{I} \]

Then, clearly

\[ P_1 \, |1, M\rangle = \frac{1}{2} S(S+1) \hat{I} \, |1, M\rangle = |1, M\rangle \]

\[ P_1 \, |0, M\rangle = \frac{1}{2} S(S+1) \hat{I} \, |1, M\rangle = 0 \]

\[ P_0 \, |1, M\rangle = \left( 1 - \frac{1}{2} S(S+1) \right) \hat{I} \, |1, M\rangle = 0 \]

\[ P_0 \, |0, M\rangle = \left( 1 - \frac{1}{2} S(S+1) \right) \hat{I} \, |0, M\rangle = |0, M\rangle \]

which are the correct properties for the projection operators.

Note also that \( P_0 = 1 - P_1 \) or \( P_0 + P_1 = 1 \) and \( P_1^2 = P_1 \) and \( P_0^2 = P_0 \) which are also correct properties for projection operators.

9.7.53 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.
This Hamiltonian is diagonal in the $|S, M\rangle$ representation. We write

$$H = A + \frac{J}{2\hbar} (S^2 - S_1^2 - S_2^2) + B \frac{S_z}{\hbar}$$

or in the $|S, M\rangle$ representation

$$H = A + \frac{J}{2} (S(S + 1) - S_1(S_1 + 1) - S_2(S_2 + 1)) + BM$$

In the case, $S_1 = 1$ and $S_2 = 1/2$, the energy eigenvalues are

$$E(S, M) = A - \frac{15}{8} J + \frac{J}{2} S(S + 1) + BM$$

Coupling the two spins we have the allowed values of $S$:

$$\frac{1}{2} \otimes 1 = \frac{1}{2} \oplus \frac{3}{2}$$

so we have

$$S = \frac{3}{2} \text{ with } M = \pm \frac{3}{2} \pm \frac{1}{2}$$

and

$$S = \frac{1}{2} \text{ with } M = \pm \frac{1}{2}$$

The final energy levels are

$$E(3/2, 3/2) = A + \frac{3}{2} B$$
$$E(3/2, 1/2) = A + \frac{1}{2} B$$
$$E(3/2, -1/2) = A - \frac{1}{2} B$$
$$E(3/2, -3/2) = A - \frac{3}{2} B$$
$$E(1/2, 1/2) = A - \frac{3}{2} J + \frac{1}{2} B$$
$$E(1/2, -1/2) = A - \frac{3}{2} J - \frac{1}{2} B$$

A plot (for $A = 10, J = 4$) as a function of $B$ is shown below:
9.7.54 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.

When coupling $\ell = 2$ and $s = 1/2$ we have

\[
\frac{1}{2} \otimes 2 = \frac{3}{2} \oplus \frac{5}{2}
\]

Therefore, we have

\[
J = \frac{5}{2} \text{ with } M = \frac{5}{2}, \frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}
\]

and

\[
J = \frac{3}{2} \text{ with } M = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}
\]

(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.

Starting with the $|5/2, 5/2\rangle$ state and using the lowering operator twice
we obtain
\[ |5/2, 1/2⟩ = \sqrt{\frac{2}{5}} |1, -1/2⟩ + \sqrt{\frac{3}{5}} |0, +1/2⟩ \]

Then, using orthogonality we get
\[ |3/2, 1/2⟩ = \sqrt{\frac{3}{5}} |1, -1/2⟩ - \sqrt{\frac{2}{5}} |0, +1/2⟩ \]

9.7.55 The Rotation Operator for Spin $-1/2$

We learned that the operator
\[ R_n(\Theta) = e^{-i\Theta(\hat{s}_n \cdot \hat{J})/\hbar} \]

is a rotation operator, which rotates a vector about an axis $\hat{e}_n$ by an angle $\Theta$. For the case of spin $1/2$,
\[ \hat{J} = \hat{S} = \frac{\hbar}{2} \hat{\sigma} \rightarrow R_n(\Theta) = e^{-i\Theta\hat{s}_n/2} \]

(a) Show that for spin $1/2$
\[ R_n(\Theta) = \cos \left( \frac{\Theta}{2} \right) \hat{I} - i \sin \left( \frac{\Theta}{2} \right) \hat{\sigma}_n \]

We have
\[ R_n(\Theta) = \sum_{m=0}^{\infty} \left( -\frac{i\Theta}{2} \right)^m \frac{(\hat{s}_n)^m}{m!} \]

Now we have $(\hat{s}_n)^2 = \hat{I}$, i.e., the square of any Pauli matrix is the identity matrix. Thus, we can separate the sum into even and odd terms

\[ (\hat{s}_n)^m = \begin{cases} \hat{I} & m \text{ even} \\ \hat{\sigma}_n & m \text{ odd} \end{cases} \]

Moreover,
\[ (-i)^m = \begin{cases} (-1)^{m/2} & m \text{ even} \\ -i(-1)^{(m-1)/2} & m \text{ odd} \end{cases} \]

This implies that
\[ R_n(\Theta) = \left( \sum_{m \text{ even}} (-1)^{m/2} \left( \frac{\Theta}{2} \right)^m \frac{1}{m!} \right) \hat{I} - i \left( \sum_{m \text{ odd}} (-1)^{(m-1)/2} \left( \frac{\Theta}{2} \right)^m \frac{1}{m!} \right) \hat{\sigma}_n \]

or
\[ R_n(\Theta) = \cos \left( \frac{\Theta}{2} \right) \hat{I} - i \sin \left( \frac{\Theta}{2} \right) \hat{\sigma}_n \]
(b) Show $R_n(\Theta = 2\pi) = -\hat{I}$; Comment.

Now

$$R_n(\Theta = 2\pi) = \cos \pi \hat{I} - i \sin \pi \hat{\sigma}_n = -\hat{I}$$

Thus,

$$R_n(\Theta = 2\pi) |\psi\rangle = -|\psi\rangle$$

For any $|\psi\rangle$ describing a spin–1/2 state, this is the famous phase associated with spinors, that differentiates it from orbital angular momentum.

(c) Consider a series of rotations. Rotate about the $y$–axis by $\theta$ followed by a rotation about the $z$–axis by $\phi$. Convince yourself that this takes the unit vector along $\vec{e}_z$ to $\vec{e}_n$. Show that up to an overall phase

$$|\uparrow_n\rangle = R_z(\phi) R_y |\uparrow_z\rangle$$

We obtain a vector in the $(\theta, \phi)$ direction by first rotating about the $y$–axis by $\theta$ and then about the $z$–axis by $\phi$. We have

$$\hat{R}_y(\theta) = \cos \frac{\theta}{2} \hat{I} - i \sin \frac{\theta}{2} \hat{\sigma}_y$$

In the $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ basis we have

$$\hat{R}_y(\theta) |\uparrow_z\rangle = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}$$

Therefore,

$$\hat{R}_y(\theta) |\uparrow_z\rangle = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \cos \frac{\phi}{2} \\ \sin \frac{\phi}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \frac{\phi}{2} \\ \sin \frac{\phi}{2} \end{pmatrix}$$

Now follow this by a rotation about the $z$–axis by $\phi$ where

$$\hat{R}_z(\phi) = \cos \frac{\phi}{2} \hat{I} - i \sin \frac{\phi}{2} \hat{\sigma}_z$$
Again, in the \{ |\uparrow_z \rangle, |\downarrow_z \rangle \} basis we have

\[ \hat{R}_z(\phi) = \begin{pmatrix} \cos \frac{\phi}{2} - i \sin \frac{\phi}{2} & 0 \\ 0 & \cos \frac{\phi}{2} + i \sin \frac{\phi}{2} \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{+i\frac{\phi}{2}} \end{pmatrix} \]

Therefore,

\[ \hat{R}_z(\phi) \left( \hat{R}_y(\theta) |\uparrow_z \rangle \right) = \left( e^{-i\frac{\phi}{2}} \cos \frac{\theta}{2} \right) \left( e^{+i\frac{\phi}{2}} \sin \frac{\theta}{2} \right) \]

or neglecting an overall phase factor

\[ \hat{R}_z(\phi) \left( \hat{R}_y(\theta) |\uparrow_z \rangle \right) = \cos \frac{\theta}{2} |\uparrow_z \rangle + e^{+i\phi} \sin \frac{\theta}{2} |\downarrow_z \rangle \]

so that

\[ \hat{R}_z(\phi) \left( \hat{R}_y(\theta) |\uparrow_z \rangle \right) = |\uparrow_n \rangle \]

9.7.56 The Spin Singlet

Consider the entangled state of two spins

\[ |\Psi_{AB} \rangle = \frac{1}{\sqrt{2}} (|\uparrow_z \rangle_A \otimes |\downarrow_z \rangle_B - |\downarrow_z \rangle_A \otimes |\uparrow_z \rangle_B) \]

(a) Show that (up to a phase)

\[ |\Psi_{AB} \rangle = \frac{1}{\sqrt{2}} (|\uparrow_n \rangle_A \otimes |\downarrow_n \rangle_B - |\downarrow_n \rangle_A \otimes |\uparrow_n \rangle_B) \]

where \{ |\uparrow_n \rangle, |\downarrow_n \rangle \} are spin spin-up and spin-down states along the direction \( \vec{e}_n \). Interpret this result.

We have

\[ |\Psi_{AB} \rangle = \frac{1}{\sqrt{2}} (|\uparrow_z \rangle_A \otimes |\downarrow_z \rangle_B - |\downarrow_z \rangle_A \otimes |\uparrow_z \rangle_B) \]

This state has zero total angular momentum. It is thus rotationally invariant and we expect it to look the same, irrespective of the quantization axis. Recall from Problem 9.7.9

\[ |\uparrow_n \rangle = \cos \frac{\phi}{2} |\uparrow_z \rangle + e^{+i\phi} \sin \frac{\phi}{2} |\downarrow_z \rangle \]
\[ |\downarrow_n \rangle = \sin \frac{\phi}{2} |\uparrow_z \rangle - e^{+i\phi} \cos \frac{\phi}{2} |\downarrow_z \rangle \]

are the spin-up and spin-down states along an arbitrary quantization axis defined by polar angles \( (\theta, \phi) \).
Consider then
\[
\frac{1}{\sqrt{2}} (|\uparrow_n\rangle \otimes |\downarrow_n\rangle - |\downarrow_n\rangle \otimes |\uparrow_n\rangle)
\]
\[
= \frac{1}{\sqrt{2}} \left( (\cos \frac{\theta}{2} |\uparrow_z\rangle + e^{+i\phi} \sin \frac{\theta}{2} |\downarrow_z\rangle) \otimes (\sin \frac{\theta}{2} |\uparrow_z\rangle - e^{+i\phi} \cos \frac{\theta}{2} |\downarrow_z\rangle) \right)
\]
\[
- \frac{1}{\sqrt{2}} \left( (\sin \frac{\theta}{2} |\uparrow_z\rangle - e^{+i\phi} \cos \frac{\theta}{2} |\downarrow_z\rangle) \otimes (\cos \frac{\theta}{2} |\uparrow_z\rangle + e^{+i\phi} \sin \frac{\theta}{2} |\downarrow_z\rangle) \right)
\]
\[
= -\frac{e^{+i\phi}}{\sqrt{2}} \left( (\cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2}) |\uparrow_z\rangle \otimes |\downarrow_z\rangle - (\cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2}) |\downarrow_z\rangle \otimes |\uparrow_z\rangle \right)
\]
\[
= -e^{+i\phi} |\Psi_{AB}\rangle
\]

Thus, up to an overall phase (which is irrelevant), the singlet state is the same for all quantization axes.

(b) Show that \( \langle \Psi_{AB} | \hat{\sigma}_n \otimes \hat{\sigma}_{n'} | \Psi_{AB} \rangle = -\vec{e}_n \cdot \vec{e}_{n'} \)

Consider the correlation function \( \langle \Psi_{AB} | \hat{\sigma}_n \otimes \hat{\sigma}_{n'} | \Psi_{AB} \rangle \). Now
\[
|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle \otimes |\downarrow_z\rangle - |\downarrow_z\rangle \otimes |\uparrow_z\rangle)
\]
which implies that
\[
\hat{\sigma}_n \otimes \hat{\sigma}_{n'} |\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} (\hat{\sigma}_n |\uparrow_z\rangle \otimes \hat{\sigma}_{n'} |\downarrow_z\rangle - \hat{\sigma}_n |\downarrow_z\rangle \otimes \hat{\sigma}_{n'} |\uparrow_z\rangle)
\]

Thus,
\[
\langle \Psi_{AB} | \hat{\sigma}_n \otimes \hat{\sigma}_{n'} | \Psi_{AB} \rangle
\]
\[
= \frac{1}{2} \langle \uparrow_z | \hat{\sigma}_n | \uparrow_z \rangle \langle \downarrow_z | \hat{\sigma}_{n'} | \downarrow_z \rangle - \frac{1}{2} \langle \downarrow_z | \hat{\sigma}_n | \uparrow_z \rangle \langle \uparrow_z | \hat{\sigma}_{n'} | \downarrow_z \rangle
\]
\[
- \frac{1}{2} \langle \uparrow_z | \hat{\sigma}_n | \downarrow_z \rangle \langle \downarrow_z | \hat{\sigma}_{n'} | \uparrow_z \rangle + \frac{1}{2} \langle \downarrow_z | \hat{\sigma}_n | \downarrow_z \rangle \langle \uparrow_z | \hat{\sigma}_{n'} | \uparrow_z \rangle
\]

Now from earlier work (in the z-basis)
\[
\hat{\sigma}_n = \begin{pmatrix} \cos \theta & e^{-i\phi} \sin \theta \\ e^{i\phi} \sin \theta & \cos \theta \end{pmatrix}
\]

Therefore,
\[
\langle \Psi_{AB} | \hat{\sigma}_n \otimes \hat{\sigma}_{n'} | \Psi_{AB} \rangle
\]
\[
= \frac{1}{2} \left( -\cos \theta \cos \theta' - e^{i(\phi-\phi')} \sin \theta \sin \theta' \right)
\]
\[
- \left( -e^{-i(\phi-\phi')} \sin \theta \sin \theta' - \cos \theta \cos \theta' \right)
\]
\[
= -\left( \cos \theta \cos \theta' + \cos (\phi - \phi') \sin \theta \sin \theta' \right)
\]
Now
\[ \vec{e}_n = \cos \theta \vec{e}_z + \sin \theta (\cos \phi \vec{e}_x + \sin \phi \vec{e}_y) \]
\[ \vec{e}_{n'} = \cos \theta' \vec{e}_z + \sin \theta'(\cos \phi' \vec{e}_x + \sin \phi' \vec{e}_y) \]
so that
\[ \vec{e}_n \cdot \vec{e}_{n'} = \cos \theta \cos \theta' + \sin \theta \sin \theta' (\cos \phi \cos \phi' + \sin \phi \sin \phi') \]
\[ = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos (\phi - \phi') \]

Therefore,
\[ \langle \Psi_{AB} | \hat{\sigma}_n \otimes \hat{\sigma}_{n'} | \Psi_{AB} \rangle = -\vec{e}_n \cdot \vec{e}_{n'} \]

As we will see later, these are the famous correlations of the Bell inequalities which cannot be captured in a local hidden variable theory.

### 9.7.57 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
\[ a = \frac{\hbar^2}{me^2}, \quad E = -\frac{\hbar^2}{2ma^2\alpha^2}, \quad z = \frac{2x}{\alpha a} \]

We consider an electron confined to the \( x \)-axis that experiences an attractive force \( e^2/r^2 \). The Schrodinger equation is
\[ \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{x}\right) \psi(x, y, z) = E \psi(x, y, z) \]

(b) Solve the Schrodinger equation for \( \psi(z) \). (You might need Mathematica, symmetry arguments plus some properties of the Confluent Hypergeometric functions or you could recognize the equation from previous work).

We can separate variables to obtain
\[ \psi(x, y, z) = \psi_n(x) \varphi_y(y) \varphi_z(z) \]
\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi_n(x)}{dx^2} - \frac{e^2}{x} \psi_n(x) = E_x \psi_n(x) \]
\[ -\frac{\hbar^2}{2m} \frac{d^2 \varphi_y(y)}{dy^2} = \frac{p_y^2}{2m} \varphi_y(y), \quad -\frac{\hbar^2}{2m} \frac{d^2 \varphi_z(z)}{dz^2} = \frac{p_z^2}{2m} \varphi_z(z) \]
\[ E = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + E_x = E_x \]

since confinement to the \( x \)-axis means that \( p_y = p_z = 0 \). This leaves us with the equation:
\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi_n(x)}{dx^2} - \frac{e^2}{x} \psi_n(x) = E_x \psi_n(x) \]

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We can rewrite this as follows (using the above definitions of constants):

\[
\frac{d^2 \psi_n(z)}{dz^2} + \frac{1}{z} \psi_n(z) = \frac{1}{4} \psi_n(z)
\]

Alternatively, we can recognize that a hydrogen-like atom of nuclear charge \( Z \) has the radial equation for \( R9r \) = \( \chi(r)/r \)

\[
-\frac{\hbar^2}{2m} \frac{d^2 \chi}{dr^2} - \frac{Ze^2}{r} \chi + \frac{\ell(\ell + 1)\hbar^2}{2mr^2} \chi = E\chi
\]

Now when \( \ell = 0 \), we have

\[
-\frac{\hbar^2}{2m} \frac{d^2 \chi}{dr^2} - \frac{Ze^2}{r} \chi = E\chi
\]

which is identical to our equation in this problem if we choose

\[
r \to x, \quad Z = 1
\]

Therefore, the ground state solution is

\[
\psi_1(x) = xR_{10}(x) = 2x \left( \frac{1}{a} \right)^{3/2} e^{-x/a}, \quad a = \frac{\hbar^2}{me^2}
\]

The ground state energy due to the \( x \)-motion is then

\[
E_x = -\frac{me^4}{2\hbar^2} = -\frac{me^4}{2\hbar^2} = -\frac{e^2}{2a}
\]

(c) Find the three lowest allowed values of energy and the corresponding bound state wavefunctions. Plot them for suitable parameter values.

The complete energy eigenvalue spectrum for the quantum state \( n \) is

\[
E_n = -\frac{e^2}{2a} \frac{1}{n^2}
\]

with wave function

\[
\psi_n(x) = AR_{n0}(x)
\]

where \( A \) is the normalization factor.

9.7.58 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 \( \ell \) quantum number for this electron?

The general solution for the Schrodinger equation of the hydrogen atom is
\[
\psi(r, \theta, \phi) = N R_{n\ell}(r) Y_{\ell m}(\theta, \phi)
\]
where
\[
H \psi(r, \theta, \phi) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r, \theta, \phi) - \frac{e^2}{r} \psi(r, \theta, \phi) = E \psi(r, \theta, \phi)
\]
and
\[
\hat{L}^2 Y_{\ell m}(\theta, \phi) = \ell(\ell + 1)\hbar^2 Y_{\ell m}(\theta, \phi)
\]
\[
\hat{L}_z Y_{\ell m}(\theta, \phi) = m\hbar Y_{\ell m}(\theta, \phi)
\]
and \( N \) is a normalization constant.

We have
\[
\psi(r, \theta, \phi) = \sqrt{\frac{3}{4\pi}} R_{n\ell}(r) Y_{10}(\theta, \phi)
\]
Therefore \( \ell = 1 \) and this is a solution for quantum numbers \((n, 1, 0)\).

Alternatively, we can calculate
\[
\hat{L}^2 \psi_{pz} = \hat{L}^2 \sqrt{\frac{3}{4\pi}} R_{n\ell}(r) \cos \theta
\]
\[
= -\sqrt{\frac{3}{4\pi}} R_{n\ell}(r) \hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \cos \theta
\]
\[
= -\sqrt{\frac{3}{4\pi}} R_{n\ell}(r) \hbar^2 \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \cos \theta}{\partial \theta} \right)
\]
\[
- \sqrt{\frac{3}{4\pi}} R_{n\ell}(r) \hbar^2 \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin^2 \theta)
\]
\[
= 2\hbar^2 \sqrt{\frac{3}{4\pi}} R_{n\ell}(r) \cos \theta = 2\hbar^2 \psi_{pz}.
\]
(b) In general, for an electron with this \( \ell \) quantum number, what are the allowed values of \( m_\ell \)? (NOTE: you should not restrict yourself to a \( p_z \) electron here). What are the allowed values of \( s \) and \( m_s \)?

\( m = m_\ell \) can always take the values \(-\ell, -\ell + 1, \ldots, +\ell\). In this case, \( m_\ell = -1, 0 \) or 1. For the electron in this problem, \( s = 1/2 \) and \( m_s = \pm 1/2 \).
(c) Write down the 6 possible pairs of $m_s$ and $m_\ell$ values for a single electron in a $p$–orbital. Given the Clebsch-Gordon coefficients shown in the table below

| $m_{j_1}$ | $m_{j_2}$ | $|j,m_j\rangle$ | $|j,m_j\rangle$ | $|j,m_j\rangle$ | $|j,m_j\rangle$ | $|j,m_j\rangle$ |
|-----------|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 1         | 1/2       | 3/2, 3/2       | 3/2, 1/2       | 1/2, 1/2       | 3/2, −1/2      | 1/2, −1/2       |
| 1         | −1/2      | 1               |                 |                 |                 |                 |
| 0         | 1/2       | $\sqrt{1/3}$   | $\sqrt{2/3}$   |                 |                 |                 |
| 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 $j_2 = 1/2$

write down all allowed coupled states $|j, m_j\rangle$ in terms of the uncoupled states $|m_\ell, m_s\rangle$. To get started here are the first three:

$|3/2, 3/2\rangle = |1, 1/2\rangle$

$|3/2, 1/2\rangle = \sqrt{2/3}|0, 1/2\rangle + \sqrt{1/3}|1, −1/2\rangle$

$|1/2, 1/2\rangle = −\sqrt{1/3}|0, 1/2\rangle + \sqrt{2/3}|1, −1/2\rangle$

For a single electron in a $p$ orbital, the following pairs of $m_\ell, m_s$ are allowed:

<table>
<thead>
<tr>
<th>$m_\ell$</th>
<th>$m_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1/2</td>
</tr>
<tr>
<td>1</td>
<td>−1/2</td>
</tr>
<tr>
<td>0</td>
<td>1/2</td>
</tr>
<tr>
<td>0</td>
<td>−1/2</td>
</tr>
<tr>
<td>−1</td>
<td>1/2</td>
</tr>
<tr>
<td>−1</td>
<td>−1/2</td>
</tr>
</tbody>
</table>

Using the Clebsch-Gordon coefficients the coupled states $|j, m_j\rangle$ are given by

$|3/2, 3/2\rangle = |1, 1/2\rangle$

$|3/2, 1/2\rangle = \sqrt{2/3}|0, 1/2\rangle + \sqrt{1/3}|1, −1/2\rangle$

$|1/2, 1/2\rangle = −\sqrt{1/3}|0, 1/2\rangle + \sqrt{2/3}|1, −1/2\rangle$

$|1/2, −1/2\rangle = \sqrt{1/3}|0, −1/2\rangle − \sqrt{2/3}|−1, 1/2\rangle$

$|3/2, −1/2\rangle = \sqrt{2/3}|0, −1/2\rangle + \sqrt{1/3}|−1, 1/2\rangle$

$|3/2, −3/2\rangle = |−1, −1/2\rangle$
(d) The spin-orbit coupling Hamiltonian, \( \hat{H}_{\text{so}} \) is given by

\[
\hat{H}_{\text{so}} = \xi(\vec{r}) \hat{\ell} \cdot \hat{s}
\]

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 ....).

There are two ways to approach this part.

**First Method:** We write

\[
\hat{H}_{\text{so}} = \xi(\vec{r}) \hat{\ell} \cdot \hat{s} = \xi(\vec{r}) \left( \hat{\ell}_z \hat{s}_z + \frac{1}{2} (\hat{\ell}_+ \hat{s}_- + \hat{\ell}_- \hat{s}_+) \right)
\]

Then, operating on the \( |j, m_j\rangle \) states written in the \( |m + \ell, m_s\rangle \) basis, we get

\[
\hat{H}_{\text{so}} |3/2, 3/2\rangle = \xi(\vec{r}) \left( \hat{\ell}_z \hat{s}_z + \frac{1}{2} (\hat{\ell}_+ \hat{s}_- + \hat{\ell}_- \hat{s}_+) \right) |1, 1/2\rangle
\]

\[
= \xi(\vec{r}) (\hbar/2) |3/2, 3/2\rangle = \frac{\hbar^2}{2} \xi(\vec{r}) |3/2, 3/2\rangle
\]

Thus, the state \( |3/2, 3/2\rangle \) is an eigenstate of \( \hat{H}_{\text{so}} \) with eigenvalue \( \hbar^2 \xi(\vec{r})/2 \).

Continuing we have

\[
\hat{H}_{\text{so}} |3/2, 1/2\rangle = \xi(\vec{r}) \left( \hat{\ell}_z \hat{s}_z + \frac{1}{2} (\hat{\ell}_+ \hat{s}_- + \hat{\ell}_- \hat{s}_+) \right) \left( \sqrt{2/3} |0, 1/2\rangle + \sqrt{1/3} |1, -1/2\rangle \right)
\]

\[
= \xi(\vec{r}) \left( \hat{\ell}_z \hat{s}_z + \frac{1}{2} (\hat{\ell}_+ \hat{s}_- + \hat{\ell}_- \hat{s}_+) \right) \left( \sqrt{2/3} |0, 1/2\rangle \right)
\]

\[
+ \xi(\vec{r}) \left( \hat{\ell}_z \hat{s}_z + \frac{1}{2} (\hat{\ell}_+ \hat{s}_- + \hat{\ell}_- \hat{s}_+) \right) \left( \sqrt{1/3} |1, -1/2\rangle \right)
\]

\[
= \frac{\hbar^2}{2} \xi(\vec{r}) \left( \sqrt{2/3} |0, 1/2\rangle + \sqrt{1/3} |1, -1/2\rangle \right) = \frac{\hbar^2}{2} \xi(\vec{r}) |3/2, 1/2\rangle
\]

Thus, the state \( |3/2, 1/2\rangle \) is an eigenstate of \( \hat{H}_{\text{so}} \) with eigenvalue \( \hbar^2 \xi(\vec{r})/2 \).

Similarly, the states \( |3/2, -1/2\rangle \) and \( |3/2, -3/2\rangle \) are also eigenstates of \( \hat{H}_{\text{so}} \) with eigenvalue \( \hbar^2 \xi(\vec{r})/2 \).

Finally,

\[
\hat{H}_{\text{so}} |1/2, 1/2\rangle = \xi(\vec{r}) \left( \hat{\ell}_z \hat{s}_z + \frac{1}{2} (\hat{\ell}_+ \hat{s}_- + \hat{\ell}_- \hat{s}_+) \right) \left( -\sqrt{1/3} |0, 1/2\rangle + \sqrt{2/3} |1, -1/2\rangle \right)
\]

\[
= -\hbar^2 \xi(\vec{r}) (-\sqrt{1/3} |0, 1/2\rangle + \sqrt{2/3} |1, -1/2\rangle) = -\hbar^2 \xi(\vec{r}) |1/2, 1/2\rangle
\]

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Thus, the state $|1/2, 1/2\rangle$ is an eigenstates of $\hat{H}_{so}$ with eigenvalue $-\hbar^2 \xi(\vec{r})$.

Similarly, the state $|1/2, -1/2\rangle$ is an eigenstates of $\hat{H}_{so}$ with eigenvalue $-\hbar^2 \xi(\vec{r})$.

**Second Method**: We write

$$\hat{j}^2 = (\hat{l} + \hat{s})^2 = \hat{l}^2 + \hat{s}^2 + 2 \hat{l} \cdot \hat{s}$$

so that

$$\hat{l} \cdot \hat{s} = \frac{1}{2}(\hat{j}^2 - \hat{l}^2 - \hat{s}^2)$$

Then, since all the states have simultaneously well-defined values of $j$, $\ell$, and $s$, they are all eigenstates of $\hat{j}^2$, $\hat{l}^2$, and $\hat{s}^2$ and hence of $\hat{H}_{so}$. To find the eigenvalues we just operate on a general state

$$\hat{H}_{so} |j, m_j\rangle = \frac{\xi(\vec{r})}{2} (\hat{j}^2 - \hat{l}^2 - \hat{s}^2) |j, m_j\rangle$$

$$= \frac{\hbar^2 \xi(\vec{r})}{2} (j(j+1) - \ell(\ell+1) - s(s+1)) |j, m_j\rangle$$

$$= \frac{\hbar^2 \xi(\vec{r})}{2} (j(j+1) - 11/4) |j, m_j\rangle$$

(9.7)

since $\ell = 1, s = 1/2$ for all these single electron $p$ orbital states.

For $j = 3/2$, we have the eigenvalue $\hbar^2 \xi(\vec{r})/2$ as before and similarly for $j = 1/2$ we have the eigenvalue $-\hbar^2 \xi(\vec{r})$ as before.

We see that the eigenvalue of $\hat{H}_{so}$ depends on the $j$ quantum number (for a given $\ell$ and $s$), i.e., it depends on how $\ell$ and $s$ are oriented relative to each other! It does not depend on $m_j$, i.e., it does not depend on the orientation of $j$.

(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

$$R_{n\ell}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \frac{1}{2\sqrt{6}} \rho e^{-\rho/2}$$

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(where \( \rho = Zr/a_0 \) and \( a_0 = 4\pi\varepsilon_0\hbar^2/m_ec^2 \)) derive an expression for the spin-orbit coupling constant for an electron in a \( 2p \)-orbital. Comment on the dependence on the atomic number \( Z \).

We need to calculate

\[
\int_0^\infty \xi(r)|R_{21}(r)|^2 r^2 dr = \frac{Ze^2}{8\pi\varepsilon_0 m_e^2 c^2} \int_0^\infty \frac{1}{r^3} |R_{21}(r)|^2 r^2 dr \\
= \frac{Ze^2}{8\pi\varepsilon_0 m_e^2 c^2} \frac{1}{24} \left( \frac{Z}{a_0} \right)^5 \int_0^\infty r e^{-Zr/a_0} dr \\
= \frac{Ze^2}{8\pi\varepsilon_0 m_e^2 c^2} \frac{1}{24} \left( \frac{Z}{a_0} \right)^3 \\
= \frac{m_e e^8}{1536\varepsilon_0 c^2 \pi \hbar^6} Z^4
\]

i.e., the strength of the SO coupling increases markedly with the atomic number (it is \( \propto Z^4 \)) which means that it is very important for heavy atoms.

(f) In the presence of a small magnetic field, \( B \), the Hamiltonian changes by a small perturbation given by

\[
\hat{H}^{(1)} = \mu_B B (\hat{l}_z + 2\hat{s}_z)
\]

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

\[
E^{(1)} = \mu_B B g_j m_j 
\]

and find the values of \( g_j \). We will prove the perturbation theory result in the Chapter 10.

We have

\[
E^{(1)} = \langle j, m_j | \mu_B B (\hat{l}_z + 2\hat{s}_z) | j, m_j \rangle
\]

To do the calculation, we rewrite the \( |j, m_j\rangle \) states in the \( |m_\ell, m_s\rangle \) basis.

Then we have for \( |j, m_j\rangle = |3/2, 3/2\rangle = |1, 1/2\rangle 

\[
E^{(1)} = \langle 1, 1/2 | \mu_B B (\hat{l}_z + 2\hat{s}_z) | 1, 1/2 \rangle = 2\hbar \mu_B B \\
= \mu_B B \frac{4}{3} \hbar m_j = \mu_B B g_j \hbar m_j
\]

with \( g_j = \frac{4}{3} \hbar \).
Similarly, we have for \(|j, m_j\rangle = |3/2, 1/2\rangle = \sqrt{3}/3 |0, 1/2\rangle + \sqrt{1/3} |1, -1/2\rangle

\[ E(1) = \mu_B \left( \frac{2}{3} (0, 1/2) \hat{l}_z + 2\hat{s}_z |0, 1/2\rangle + \frac{1}{3} (1, -1/2) \hat{l}_z + 2\hat{s}_z |1, -1/2\rangle \right) \]

\[ = \mu_B \left( \frac{2}{3} \hbar + \frac{1}{3} (0) \right) = \mu_B B \frac{4}{3} \hbar m_j = \mu_B B g_j m_j \text{ with } g_j = \frac{4}{3} \hbar \]

Similarly, we get for \(|j, m_j\rangle = |1/2, 1/2\rangle = \sqrt{1/3} |0, 1/2\rangle + \sqrt{2/3} |1, -1/2\rangle

\[ E(1) = \mu_B B g_j m_j \text{ with } g_j = \frac{2}{3} \hbar \]

So, in general we have

\[ g_j = \frac{1}{3} (2j + 1) \hbar \text{ and } E(1) = \frac{1}{3} m_j (2j + 1) \hbar \mu_B B \]

(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.

Assuming that the energy splitting resulting from the spin-orbit coupling is larger than that due to the magnetic field, we have the following energy level diagram:
Note that at zero field \((j = 3/2, m_j = \pm 3/2, \pm 1/2)\) are degenerate and \((j = 1/2, m_j = \pm 1/2)\) are degenerate.

### 9.7.59 Quadrupole Moment Operators

The quadrupole moment operators can be written as

\[
Q^{(+2)} = \sqrt{\frac{3}{8}} (x + iy)^2
\]
\[
Q^{(+1)} = -\sqrt{\frac{3}{2}} (x + iy)z
\]
\[
Q^{(0)} = \frac{1}{2} (3z^2 - r^2)
\]
\[
Q^{(-1)} = \sqrt{\frac{3}{2}} (x - iy)z
\]
\[
Q^{(-2)} = \sqrt{\frac{3}{8}} (x - iy)^2
\]

Using the form of the wave function \(\psi_{lm} = R(r)Y_{lm}^*(\theta, \phi)\),

(a) Calculate \(\langle \psi_{3,3} | Q^{(0)} | \psi_{3,3} \rangle\)

We need to calculate

\[
\langle \psi_{3,3} | Q_0 | \psi_{3,3} \rangle = \int dr r^2 R^2(r)r^2 \int d\Omega Y_{3,3}^*(\theta, \phi) \frac{Q_0}{r^2} Y_{3,3}(\theta, \phi)
\]
where
\[ Q_0 = \frac{1}{r^2} (3z^2 - r^2) = \frac{1}{2} (3\cos^2 \theta - 1) \]

We can ignore the radial integral (which just factors out in all cases) and compute the angular integral.

We use Mathematica. We define \( Q_0 \) and the integral:

```mathematica
q0 = \frac{1}{2} (3 \cos^2 \theta - 1);
shavq[m2_, q_, m1_] := Integrate[Conjugate[SphericalHarmonicY[3, m2, \[Theta], \[Phi]]] 
q SphericalHarmonicY[3, m1, \[Theta], \[Phi]] Sin[\[Theta]], \{\[Theta], 0, \[Pi] \}, \{\[Phi], 0, 2 \[Pi] \}];
```

and then compute

\[
q0a33 = shavq[3, q0, 3]
\]

\[
q0a33 = \frac{-1}{3}
\]

(b) Predict all others \( \langle \psi_{3,m'} | Q_0^{(0)} | \psi_{3,m} \rangle \) using the Wigner-Eckart theorem in terms of Clebsch-Gordon coefficients.

Using the result above, the double-bar-inner-product on the RHS of the Wigner-Eckhart theorem is

\[
dbavg = q0a33 / ClebschGordan[{3, 3}, {2, 0}, {3, 3}] * \sqrt{\frac{7}{15}}
\]

\[
-2 \sqrt{\frac{7}{15}}
\]

Then, we can insert this in a general function for any \( m_1 \) and \( m_2 \):

```mathematica
weavq[m2_, q_, m1_] := ClebschGordan[{3, m1}, {2, q}, {3, m2}] * dbavg / \sqrt{7};
```

or written out...

\[
\langle 3, m_2 | (Q_0^{(2)})_q | 3, m_1 \rangle = \left( \frac{1}{\sqrt{7}} \right) \langle 3, 2; m_1, q | 3, 2 : 3, m_2 \rangle \left( -2 \sqrt{\frac{7}{15}} \right)
\]

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On the RHS, the first factor comes from $1/\sqrt{2j_1 + 1}$ where $j_1 = 3$ is the total angular momentum eigenvalue of the ket.

The second factor is the Clebsch-Gordon coefficient of

$$|j_1, m_1\rangle \otimes |k, q\rangle \leftrightarrow |j_2, m_2\rangle$$

For this problem, $j_1 = j_2 = 3$ and we get a non-zero result only if $m_1 + q = m_2$ and $|j_1 - j_2| < k < j_1 + j_2$, which is satisfied since $k = 2$ for the quadrupole tensor.

The third factor is shown to exist by the Wigner-Eckhart theorem is $\langle 3\|Q\|3 \rangle$. It is independent of the quantum numbers $m_1, m_2$ and $q$, depending only on the quantum numbers $j_1, j_2$ and $k$.

(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 $\langle \psi_{3,-2} | Q^{(0)} | \psi_{3,-3} \rangle$.

Let us define the $Q$ operators in similar fashion to (a):

$$q_{p1} = -\sqrt{\frac{3}{2}} (\sin[\theta] \cos[\phi] + i \sin[\theta] \sin[\phi]) \cos[\theta];$$

$$q_{m2} = \sqrt{\frac{3}{8}} (\sin[\theta] \cos[\phi] - i \sin[\theta] \sin[\phi])^2;$$

and compute the inner products using the $\text{shavg}$ function from (a):

```
\text{shavg}[1, q_{p1}, 0]
\text{shavg}[-1, q_{m2}, 1]
\text{shavg}[-2, q_{00}, -3]
```

\[
\frac{\sqrt{2}}{15}
\]

\[
-\frac{2\sqrt{2}}{3}
\]

\[
0
\]
Note that we leave \( r^2 = \int_0^\infty r^2 \, dr R^2(r) r^2 \) as an overall constant that drops out from the ratios.

Compare the results using the Wigner-Eckhart function from (b):

\[
\begin{align*}
\text{weavg}[1, 1, 0] \\
\text{weavg}[1, -2, 1] \\
\text{weavg}[2, 0, -3]
\end{align*}
\]

\[
\begin{align*}
\frac{\sqrt{2}}{15} \\
- \frac{2\sqrt{2}}{5}
\end{align*}
\]

ClebschGordan::phy : ThreeJSymbol[{3, -3}, {2, 0}, {3, 2}] is not physical. More...

0

9.7.60 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 \( |j, m\rangle = |5/2, 5/2\rangle = |3/2, 3/2\rangle \otimes |1, 1\rangle \).

We have the relationship

\[
J_\pm |j_1 j_2; jm\rangle = (J_1 \pm J_2) \sum_{m_1} \sum_{m_2} |j_1 j_2; m_1 m_2\rangle \langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle
\]

where

\[
C(j_1 j_2; m_1 m_2) = \langle j_1 j_2; m_2 m_2 | j_1 j_2; jm\rangle = \text{Clebsch-Gordon coefficient}
\]

Expanding out we have

\[
\sqrt{(j \pm m)(j \pm m + 1)} |j_1 j_2; jm \pm 1\rangle = \sum_{m'_1} \sum_{m'_2} \sqrt{(j_1 \pm m'_1)(j_1 \pm m'_1 + 1)} |j_1 j_2; m'_1 \pm 1, m'_2\rangle \langle j_1 j_2; m'_1 m'_2 | j_1 j_2; jm\rangle
\]

\[
+ \sum_{m'_1} \sum_{m'_2} \sqrt{(j_2 \pm m'_2)(j_2 \pm m'_2 + 1)} |j_1 j_2; m'_1, m'_2 \pm 1\rangle \langle j_1 j_2; m'_1 m'_2 | j_1 j_2; jm\rangle
\]

Using orthonormality, we take the scalar product with \( \langle j_1 j_2; m_1 m_2\rangle \) and find that the first term on the RHS contributes only if \( m_1 = m'_1 \pm 1 \) and \( m_2 = m'_2 \) and the second term on the RHS contributes only if \( m_1 = m'_1 \) and \( m_2 = m'_2 \pm 1 \).
Therefore we get the recursion relation:

\[
\sqrt{(j \mp m)(j \pm m + 1)} C(j_1 j_2; m_1, m_2, m) = \sqrt{(j_1 \mp m_1 + 1)(j_1 \pm m_1)} C(j_1 j_2; m_1 \mp 1, m_2, m)
\]

\[
+ \sqrt{(j_2 \mp m_2 + 1)(j_2 \pm m_2)} C(j_1 j_2; m_1, m_2 \mp 1, m)
\]

where now \( m_1 + m_2 = m \pm 1 \). An example of its use is shown below. For \( j = 5/2, m = 5/2 \) we have using the lower sign

\[
\sqrt{5} C(3/2, 1, 5/2; 3/2, 0, 3/2) = \sqrt{2} C(3/2, 1, 5/2; 3/2, 1, 5/2)
\]

By convention \( C(3/2, 1, 5/2; 3/2, 1, 5/2) = 1 \). Therefore we obtain

\[
C(3/2, 1, 5/2; 3/2, 0, 3/2) = \sqrt{2} \frac{2}{5}
\]

and

\[
\sqrt{5} C(3/2, 1, 5/2; 1/2, 1, 3/2) = \sqrt{5} C(3/2, 1, 5/2; 3/2, 1, 5/2)
\]

so that

\[
C(3/2, 1, 5/2; 1/2, 1, 3/2) = \frac{3}{5}
\]

and therefore

\[
|3/2; 5/2, 3/2\rangle = C(3/2, 1, 5/2; 1/2, 1, 3/2) |3/2, 1; 1/2, 1\rangle
\]

\[
+ C(3/2, 1, 5/2; 3/2, 0, 3/2) |3/2, 1; 3/2, 0\rangle
\]

or

\[
|3/2; 5/2, 3/2\rangle = \sqrt{\frac{3}{5}} |3/2, 1; 1/2, 1\rangle + \sqrt{\frac{2}{5}} |3/2, 1; 3/2, 0\rangle
\]

This leads to the following sequence using Mathematica. We implement the lowering eigenvalue

\[
\text{lower}[j_, m_] = \sqrt{(j + m)(j - m + 1)}
\]

Then we start from the maximum state \( j = 5/2, m = 5/2 \) and write for \( m = 3/2 \):
Thus we get (as before)

\[ C(3/2, 1, 5/2; 1/2, 1, 3/2) = \sqrt{3/5} \]
\[ C(3/2, 1, 5/2; 3/2, 0, 3/2) = \sqrt{2/5} \]

Then for \( m = 1/2 \):

\[ \sqrt{3/5 \, \text{lower}[3/2, 1/2] / \text{lower}[5/2, 3/2]} \]
\[ \sqrt{3/5 \, \text{lower}[1, 1] / \text{lower}[5/2, 3/2]} \]
\[ \sqrt{2/5 \, \text{lower}[3/2, 3/2] / \text{lower}[5/2, 3/2]} \]
\[ \sqrt{2/5 \, \text{lower}[1, 0] / \text{lower}[5/2, 3/2]} \]
\[ \sqrt{3/10} \]
\[ \sqrt{2/5} \]
\[ \sqrt{2/5} \]
\[ \sqrt{1/10} \]

so that we get

\[ C(3/2, 1, 5/2; -1/2, 1, 1/2) = \sqrt{3/10} \]
\[ C(3/2, 1, 5/2; 1/2, 0, 1/2) = \frac{1}{2} \sqrt{3/5} + \frac{1}{2} \sqrt{3/5} = \sqrt{3/5} \]
\[ C(3/2, 1, 5/2; 3/2, -1, 1/2) = \sqrt{1/10} \]

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Note that the second and third terms end up as \(|3/2, 1/2\) \(\otimes\) \(|1, 0\) and we just add their contributions.

Then for \(m = -1/2\):

\[
\begin{align*}
\sqrt{3/10} & \text{ lower}[3/2, -1/2] / \text{ lower}[5/2, 1/2] \\
\sqrt{3/10} & \text{ lower}[1, 1] / \text{ lower}[5/2, 1/2] \\
\sqrt{3/5} & \text{ lower}[3/2, 1/2] / \text{ lower}[5/2, 1/2] \\
\sqrt{3/5} & \text{ lower}[1, 0] / \text{ lower}[5/2, 1/2] \\
\sqrt{1/10} & \text{ lower}[3/2, 3/2] / \text{ lower}[5/2, 1/2] \\
\frac{1}{\sqrt{10}} \\
\frac{1}{\sqrt{15}} \\
\frac{2}{\sqrt{15}} \\
\sqrt{\frac{2}{15}} \\
\frac{1}{\sqrt{30}}
\end{align*}
\]

so that

\[
\begin{align*}
C(3/2, 1, 5/2; -3/2, 1, -1/2) &= \sqrt{\frac{1}{10}} \\
C(3/2, 1, 5/2; -1/2, 0, -1/2) &= \sqrt{\frac{1}{15}} + 2\sqrt{\frac{1}{15}} = \sqrt{\frac{3}{5}} \\
C(3/2, 1, 5/2; 1/2, -1, -1/2) &= \sqrt{\frac{2}{15}} + \sqrt{\frac{1}{30}} = \sqrt{\frac{3}{10}}
\end{align*}
\]

Note that we omitted the term which would have lowered \(|1, -1\).

Then for \(m = -3/2\):
so that

\[
\begin{align*}
\sqrt{\frac{1}{10}} \text{lower}[1, 1]/\text{lower}[5/2, -1/2] \\
\sqrt{\frac{3}{5}} \text{lower}[3/2, -1/2]/\text{lower}[5/2, -1/2] \\
\sqrt{\frac{3}{5}} \text{lower}[1, 0]/\text{lower}[5/2, -1/2] \\
\sqrt{\frac{3}{10}} \text{lower}[3/2, 1/2]/\text{lower}[5/2, -1/2] \\
\frac{1}{2} \sqrt{\frac{10}{10}} \\
\frac{3}{2} \sqrt{\frac{10}{10}} \\
\frac{\sqrt{5}}{2} \\
\frac{\sqrt{3}}{2}
\end{align*}
\]

so that

\[
\begin{align*}
C(3/2, 1, 5/2; -3/2, 0, -3/2) &= \frac{1}{2} \sqrt{\frac{1}{10}} + \frac{1}{2} \sqrt{\frac{9}{10}} = \sqrt{\frac{2}{5}} \\
C(3/2, 1, 5/2; 1/2, -1, -1/2) &= \frac{1}{2} \sqrt{\frac{3}{5}} + \frac{1}{2} \sqrt{\frac{3}{5}} = \sqrt{\frac{3}{5}}
\end{align*}
\]

Here we omitted two terms due to annihilation. Note that the results are the same as with \(|5/2, 3/2\rangle\), which one expects by symmetry.

Finally, for \(m = -5/2\):

\[
\begin{align*}
\sqrt{\frac{2}{5}} \text{lower}[1, 0]/\text{lower}[5/2, -3/2] \\
\sqrt{\frac{3}{5}} \text{lower}[3/2, -1/2]/\text{lower}[5/2, -3/2] \\
\frac{2}{5} \\
\frac{3}{5}
\end{align*}
\]
so that

\[ C(3/2, 1, 5/2; -3/2, -1, -5/2) = \frac{2}{5} + \frac{3}{5} = 1 \]

This is necessary by both convention and symmetry.

We have now completed all the n-n-zero CG coefficients for \( j = 5/2 \). We are not done, however, we must calculate the CG coefficients for \( j = 3/2 \) and \( j = 1/2 \) representations also. Unfortunately, there is no single extreme states to start the process. What are we to do?

Now, we know that the different representations we get when adding angular momentum are separate and irreducible, so eigenstates from different representations with the same \( m \) eigenvalue must be orthogonal. Indeed the number of ways to produce a particular \( m \) states with \( |j_1m_1⟩ \otimes |j_2m_2⟩ \) is equal to the number of irreducible representations.

Knowing this, we can immediately write down the the CG coefficients for the mainum \( m \) state of the sum representation \( j = 3/2, |3/3, 3/2⟩ \):

\[ C(3/2, 1, 3/2; 1/2, 1, 3/2) = -\sqrt{\frac{2}{5}} \]

\[ C(3/2, 1, 3/2; 3/2, 0, 3/2) = \sqrt{\frac{3}{5}} \]

Note that we have fixed a sign convention.

We can now proceed in the same fashion as before. First, for \( m = 1/2 \):

\[
\begin{align*}
-\sqrt{\frac{2}{5}} \text{ lower}[3/2, 1/2] & / \text{ lower}[3/2, 3/2] \\
-\sqrt{\frac{2}{5}} \text{ lower}[1, 1] & / \text{ lower}[3/2, 3/2] \\
\sqrt{\frac{3}{5}} \text{ lower}[3/2, 3/2] & / \text{ lower}[3/2, 3/2] \\
\sqrt{\frac{3}{5}} \text{ lower}[1, 0] & / \text{ lower}[3/2, 3/2] \\
-2 \sqrt{\frac{2}{15}} & \\
\frac{2}{\sqrt{15}} & \\
\sqrt{\frac{3}{5}} & \\
\sqrt{\frac{2}{5}} & 
\end{align*}
\]
so that

\[
C(3/3, 1, 3/2; -1/2, 1, 1/2) = -\sqrt{\frac{8}{15}} \\
C(3/3, 1, 3/2; 1/2, 0, 1/2) = -2\sqrt{\frac{1}{15}} + 3\sqrt{\frac{1}{15}} = \sqrt{\frac{1}{15}} \\
C(3/3, 1, 3/2; 3/2, -1, 1/2) = -\sqrt{\frac{2}{5}}
\]

Then for \( m = -1/2 \):

\[
\begin{align*}
\sqrt{\frac{1}{15}} \text{ lower}[3/2, 1/2] / \text{ lower}[3/2, 1/2] \\
\sqrt{\frac{1}{15}} \text{ lower}[1, 0] / \text{ lower}[3/2, 1/2] \\
\sqrt{\frac{2}{5}} \text{ lower}[3/2, 3/2] / \text{ lower}[3/2, 1/2] \\
\sqrt{\frac{2}{5}} \\
\sqrt{\frac{1}{15}} \\
\sqrt{\frac{1}{15}} \\
\sqrt{\frac{1}{30}} \\
\sqrt{\frac{3}{10}}
\end{align*}
\]

so that

\[
C(3/3, 1, 3/2; -3/2, 1, -1/2) = -\sqrt{\frac{2}{5}} \\
C(3/3, 1, 3/2; -1/2, 0, -1/2) = -2\sqrt{\frac{1}{15}} + \sqrt{\frac{1}{15}} = -\sqrt{\frac{3}{5}} \\
C(3/3, 1, 3/2; 1/2, -1, -1/2) = -\frac{1}{3}\sqrt{\frac{2}{5}} + 4\sqrt{\frac{2}{5}} = \sqrt{\frac{2}{5}}
\]

One might expect this result from symmetry, taking into account the minus sign.

Finally for \( m = -3/2 \):
so that

\[
C(3/3, 1, 3/2; -3/2, 0, -3/2) = -2\sqrt{\frac{1}{15}} - \sqrt{\frac{1}{15}} = -\sqrt{\frac{1}{15}}
\]

\[
C(3/3, 1, 3/2; -1/2, -1, -3/2) = \sqrt{\frac{1}{30}} + \sqrt{\frac{9}{30}} = \sqrt{\frac{8}{15}}
\]

Again, we could have predicted this result by symmetry.

Finally, for \( j = 1/2 \), we can again construct the \( m = 1/2 \) state, and therefore the CG coefficients, by orthogonality to both \(|5/2, 1/2\rangle\) and \(|3/2, 1/2\rangle\). Then we solve

\[
\sqrt{\frac{3}{10}} x + \sqrt{\frac{3}{5}} y + \sqrt{\frac{1}{10}} z = 0
\]

\[
-\sqrt{\frac{8}{15}} x + \sqrt{\frac{1}{15}} y + \sqrt{\frac{2}{5}} z = 0
\]

where \( x, y, z \) are the CG coefficients

\[
\text{Solve}\left[\left\{\sqrt{\frac{3}{10}} x + \sqrt{\frac{3}{5}} y + \sqrt{\frac{1}{10}} z = 0,\right.\right.
\]

\[
\left.\left. -\sqrt{\frac{8}{15}} x + \sqrt{\frac{1}{15}} y + \sqrt{\frac{2}{5}} z = 0,\quad x^2 + y^2 + z^2 = 1\right\}, \{x, y, z\}\right]\]

\[
\left\{\left[z \to \frac{1}{\sqrt{2}}, x \to -\frac{1}{\sqrt{6}}, y \to \frac{1}{\sqrt{3}}\right], \left\{z \to \frac{1}{\sqrt{2}}, x \to \frac{1}{\sqrt{6}}, y \to -\frac{1}{\sqrt{3}}\right\}\right\}
\]
to get
\[ C(3/3, 1, 3/2; -1/2, 1, 1/2) = -\sqrt{1/6} \]
\[ C(3/3, 1, 3/2; 1/2, 0, 1/2) = -\sqrt{1/3} \]
\[ C(3/3, 1, 3/2; 3/2, -1, 1/2) = \sqrt{1/2} \]

where we have chosen a sign convention.

We can do the same for \( m = -1/2 \):

\[ \text{Solve}\left[ \left\{ \sqrt{\frac{1}{10}} x + \sqrt{\frac{3}{5}} y + \sqrt{\frac{3}{10}} z = 0, \right. \right. \]
\[ \left. \left. -\sqrt{\frac{2}{5}} x - \sqrt{\frac{1}{15}} y + \sqrt{\frac{8}{15}} z = 0, \quad x^2 + y^2 + z^2 = 1 \right\}, \{ x, y, z \} \right] \]
\[ \left\{ \left\{ z \rightarrow -\frac{1}{\sqrt{6}}, \quad x \rightarrow -\frac{1}{\sqrt{2}}, \quad y \rightarrow \frac{1}{\sqrt{3}} \right\}, \left\{ z \rightarrow \frac{1}{\sqrt{6}}, \quad x \rightarrow \frac{1}{\sqrt{2}}, \quad y \rightarrow -\frac{1}{\sqrt{3}} \right\} \right\} \]

to get
\[ C(3/3, 1, 3/2; -3/2, 1, -1/2) = \sqrt{1/2} \]
\[ C(3/3, 1, 3/2; -1/2, 0, -1/2) = -\sqrt{1/3} \]
\[ C(3/3, 1, 3/2; 1/2, -1, -1/2) = \sqrt{1/6} \]

9.7.61 Spherical Harmonics Properties

Again, we will use Mathematica.

(a) Show that \( L_+ \) annihilates \( Y_2^2 = \sqrt{15}/32\pi \sin^2 \theta e^{2i\phi} \).

The raising operator in the position representation is
\[ L_+ = -i\hbar e^{i\phi} \left( i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \]

Applying it to \( Y_{22} \) we get
(b) Work out all of $Y_2^m$ using successive applications of $L_-$ on $Y_2^2$.

The lowering operator in the position representation is

$$L_- = -i\hbar e^{i\phi} \left(-i\frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi}\right)$$

We implement both it and its eigenvalue

\[
\text{lowy}[y_] := (-I\hbar) \text{Exp}[-I\phi] (-I \text{D}[y, \theta] - \text{Cot}[\theta] \text{D}[y, \phi]); \\
\text{lowyv}[m_] = \sqrt{(2 + m)(2 - m + 1)} \; \hbar;
\]

and apply it repeatedly to $Y_{22}$:

\[
y_{21} = \text{lowy}[\text{SphericalHarmonicY}[2, 2, \theta, \phi]] / \text{lowyv}[2]
\]

$$\frac{1}{2} e^{i\phi} \sqrt{\frac{15}{2\pi}} \cos[\theta] \sin[\theta]$$

$$y_{21} - \text{SphericalHarmonicY}[2, 1, \theta, \phi]$$

$$0$$
(c) Plot the shapes of $Y_2^m$ in 3-dimensions $(r, \theta, \phi)$ using $r = Y_2^m(\theta, \phi)$. 

\[ y_{20} = \text{Simplify}[\text{lows}[y_{21}] / \text{lows}[1]] \]

\[ \frac{1}{8} \sqrt{\frac{5}{\pi}} (1 + 3 \cos(2\theta)) \]

\[ \text{Simplify}[y_{20} - \text{SphericalHarmonicY}[2, 0, \theta, \phi]] \]

0

\[ y_{2m1} = \text{lows}[y_{20}] / \text{lows}[0] \]

\[ \frac{1}{4} \mathrm{e}^{-i\phi} \sqrt{\frac{15}{2\pi}} \sin(2\theta) \]

\[ \text{Simplify}[y_{2m1} - \text{SphericalHarmonicY}[2, -1, \theta, \phi]] \]

0

\[ y_{2m2} = \text{Simplify}[\text{lows}[y_{2m1}] / \text{lows}[1]] \]

\[ \frac{1}{4} \mathrm{e}^{-2i\phi} \sqrt{\frac{15}{2\pi}} \sin^2(\theta) \]

\[ \text{Simplify}[y_{2m2} - \text{SphericalHarmonicY}[2, -2, \theta, \phi]] \]

0

\[ \text{lows}[y_{2m2}] \]

0
First we create a plotting function

\[
\text{ploty}[m_] := \text{ParametricPlot3D[} \\
\quad \text{Conjugate[SphericalHarmonicY[2, m, \theta, \phi]] SphericalHarmonicY[2, m, \theta, \phi]} \\
\quad \{\text{Sin[\theta] Cos[\phi], Sin[\theta] Sin[\phi], Cos[\theta]}\}, \{\theta, 0, \pi\}, \{\phi, 0, 2\pi\}, \text{PlotPoints \rightarrow 50}\};
\]

and plot \(|Y_{2m}|^2\) for \(m = 0, 1, 2\):

\[
\text{Table[ploty}[m], \{m, 0, 2\}];
\]
There exists a really clever Mathematica notebook created by one of my former students in the Quantum Seminar at Swarthmore College. It calculates the CG coefficients for arbitrary $j_1$ and $j_2$ and then writes out the states in Dirac notation. It is located at http://chaos.swarthmore.edu/Physics1132011/clebsch-gordon.nb.zip

9.7.62 Starting Point for Shell Model of Nuclei

Consider a three-dimensional isotropic harmonic oscillator with Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2} m \omega^2 \mathbf{r}^2 = h\omega \left( \mathbf{\hat{a}}^+ \cdot \mathbf{\hat{a}} + \frac{3}{2} \right)$$

where $\mathbf{p} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$, $\mathbf{r} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$, $\mathbf{\hat{a}} = (\hat{a}_1, \hat{a}_2, \hat{a}_3)$. We also have the commutators $[\hat{x}, \hat{p}, \hat{p}] = ih\delta_{ij}$, $[\hat{x}, \hat{x}] = 0$, $[\hat{p}, \hat{p}] = 0$, $[\hat{a}, \hat{a}] = 0$, $[\hat{a}^+, \hat{a}^+] = 0$, 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 $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ commutes with
the Hamiltonian.

We handle the two terms separately; first the kinetic energy,
\[
L_i = \epsilon_{ijk} \left[ x_j p_k - \frac{p_j p_k}{2m} \right] = \epsilon_{ijk} \left[ x_j p_k + \frac{p_j p_k}{2m} \right] = \epsilon_{ijk} 2i\hbar \delta_{ij} p_i \frac{p_k}{2m} = \frac{i\hbar}{m} \epsilon_{ijk} p_j p_k = 0
\]
by the antisymmetry of \(\epsilon_{ijk}\). Similarly for the potential energy,
\[
L_i = \frac{1}{2} m \omega^2 x^2 = \epsilon_{ijk} \left[ x_j x_k \right] = \frac{1}{2} m \omega^2 \epsilon_{ijk} x_j x_k = -i\hbar \omega^2 \epsilon_{ijk} \delta_{kl} x_l = -i\hbar \omega^2 \epsilon_{ijk} x_j x_k = 0
\]
by the antisymmetry of \(\epsilon_{ijk}\).

(b) Rewrite \(\vec{L}\) in terms of creation and annihilation operators.

We generalize the usual creation and annihilation operators for each spatial direction,
\[
a_i = \sqrt{\frac{m \omega}{2\hbar}} \left( x_i + i \frac{p_i}{m \omega} \right) , \quad a_i^+ = \sqrt{\frac{m \omega}{2\hbar}} \left( x_i - i \frac{p_i}{m \omega} \right)
\]
The commutation relations are obviously \([a_i, a_j^+] = \delta_{ij}\). The Hamiltonian is simply the sum of three 1D harmonic oscillator Hamiltonians
\[
H = \hbar \omega \left( a_x^+ a_x + a_y^+ a_y + a_z^+ a_z + \frac{3}{2} \right)
\]
The angular momentum operators are rewritten using
\[
x_i = \sqrt{\frac{\hbar}{2m \omega}} (a_i + a_i^+) , \quad p_i = -i \sqrt{\frac{\hbar m \omega}{2}} (a_i - a_i^+)
\]
We find
\[
L_i = \epsilon_{ijk} x_j p_k = \epsilon_{ijk} \sqrt{\frac{\hbar}{2m \omega}} (a_j + a_j^+) \left( -i \sqrt{\frac{\hbar m \omega}{2}} (a_k - a_k^+) \right)
\]
\[
= -i \frac{\hbar}{2} \epsilon_{ijk} (a_j + a_j^+) (a_k - a_k^+)
\]
\[
= -i \frac{\hbar}{2} \epsilon_{ijk} (a_j a_k - a_j a_k^+ + a_j^+ a_k - a_j^+ a_k^+)
\]
\[
= -i \hbar \epsilon_{ijk} (a_j^+ a_k - a_k^+ a_j)
\]
\[
= -i \hbar \epsilon_{ijk} a_j^+ a_k
\]
where we have used $\epsilon_{ijk}a_ja_k = \epsilon_{ijk}a_j^+a_k^+ = 0$, $\epsilon_{ijk}\delta_{kj} = 0$ and $\epsilon_{ijk} = -\epsilon_{ikj}$.

For later purposes, it is useful to define

$$a_+ = -\frac{1}{\sqrt{2}}(a_x - ia_y), \quad a_- = \frac{1}{\sqrt{2}}(a_x + ia_y)$$

Note that

$$[a_+, a_+] = [a_, a_+] = 1$$
$$[a_+, a_-] = [a_+, a_-] = [a_+, a_-] = 0$$

Then the angular momentum operators can be further rewritten as

$$L_+ = L_x + iL_y = -i\hbar(a_y^+a_z - a_z^+a_y) + \hbar(a_x^+a_x - a_z^+a_z)$$
$$= \hbar((-a_x^+ + ia_y^+)a_x + a_z^+(a_x + ia_y))$$
$$= \hbar\sqrt{2}(a_x^+a_z + a_z^+a_-)$$

$$L_- = L_x - iL_y = -i\hbar(a_y^+a_z - a_z^+a_y) - \hbar(a_x^+a_x - a_z^+a_z)$$
$$= \hbar((a_x^+ + ia_y^+)a_z - a_z^+(a_x - ia_y))$$
$$= \hbar\sqrt{2}(a_x^+a_z + a_z^+a_+)$$

$$L_z = -i\hbar(a^+x a_y - a_y^+a_x) = -i\hbar\left(\frac{a_-^+a_+a_+}{\sqrt{2}} - \frac{a_+^+a_-a_-}{\sqrt{2}}\right)$$
$$= \hbar(a_x^+a_+ - a_x^+a_-)$$

In other words, $a_x^+(a_+)$ creates (annihilates) the excitation with $L_z = +\hbar$, while $a_x^-(a_-)$ creates (annihilates) the excitation with $L_z = -\hbar$.

(c) Show that $|0\rangle$ belongs to the $\ell = 0$ representation. It is called the 1S state.

The ground state is unique, and the only representation of angular momentum that can be formed by a single state is $\ell = 0$. A more explicit way to show it, is simply by acting

$$L_+ |0\rangle = \hbar\sqrt{2}(a_x^+a_z + a^+_za_-) |0\rangle = 0$$
$$L_- |0\rangle = \hbar\sqrt{2}(a_x^+a_z + a^+_za_+) |0\rangle = 0$$
$$L_z |0\rangle = \hbar(a_x^+a_+ - a_x^+a_-) |0\rangle = 0$$

(d) Show that the operators $\mp(a^+_1 \pm a^+_2)$ and $a_3^+$ form spherical tensor operators.
ASIDE: Definition of a spherical tensor:

We define a spherical tensor of rank \( k \) as a set of \( 2^{k+1} \) operators \( T^{q}_k \), \( q = k, k-1, ..., -k \) such that under rotation they transform among themselves with exactly the same matrix of coefficients as that for the \( 2j+1 \) angular momentum eigenkets \(|m\rangle\) for \( k = j \), that is,

\[
U(R)T^{q}_kU^+(R) = \sum_{q'} D^{(k)}_{q'q} T^{q'}_{k}
\]

To explicitly see the properties of these spherical tensors, it is useful to evaluate the above equation for infinitesimal rotations, for which

\[
D^{(k)}_{q'q}(\epsilon) = \langle k, q' | I - i\epsilon \cdot \vec{J}/\hbar | k, q \rangle = \delta_{q'q} - \epsilon \cdot \langle k, q' | \vec{J}/\hbar | k, q \rangle
\]

Specifically, consider the infinitesimal rotation \( \epsilon \cdot \vec{J} = \epsilon J^+ + \epsilon J^- \). (Strictly, speaking, this is not a real rotation, but the formalism does not care, and the result we can derive can be confirmed by rotation about the \( x \) and \( y \) directions and adding appropriate terms).

The equation is

\[
(1 - i\epsilon \frac{J^+}{\hbar}) T^{q}_k (1 + i\epsilon \frac{J^-}{\hbar}) = \sum_{q} (\delta_{q'q} - i\epsilon \langle k, q' | J^+/\hbar | k, q \rangle) T^{q'}_{k}
\]

and equating terms linear in \( \epsilon \) we have

\[
[J_{\pm}, T^{q}_k] = \pm \hbar \sqrt{(k \mp q)(k \pm q + 1)} T^{q\pm 1}_k
\]

\[
[J_z, T^{q}_k] = \hbar q T^{q}_k
\]

which can be taken as the definitions of spherical tensors. The creation operators are \( k = 1 \) spherical tensor operators.

\[
T^{(1)}_{+1} = a^+_z, \quad T^{(1)}_0 = a^+_z, \quad T^{(1)}_{-1} = a^+_z
\]

To verify this claim:

\[
[L_+, T^{(1)}_{+1}] = [\hbar \sqrt{2}(a^+_z a^-_z + a^+_z a^-_z), a^+_z] = 0
\]

\[
[L_-, T^{(1)}_{-1}] = [\hbar \sqrt{2}(a^-_z a^+_z + a^-_z a^+_z), a^+_z] = \hbar \sqrt{2} T^{(1)}_0
\]

\[
[L_-, T^{(1)}_{+1}] = [\hbar \sqrt{2}(a^-_z a^+_z + a^-_z a^+_z), a^+_z] = \hbar \sqrt{2} T^{(1)}_{-1}
\]

\[
[L_-, T^{(1)}_{-1}] = [\hbar \sqrt{2}(a^-_z a^+_z + a^-_z a^+_z), a^-_z] = 0
\]

Indeed, the operators form the \( k = 1 \) representation.

(e) Show that \( N = 1 \) states, \( |1, 1, \pm 1\rangle = (a^+_z \pm a^+_z)|0\rangle / \sqrt{2} \) and \( |1, 1, 0\rangle = a^+_z|0\rangle \), form the \( \ell = 1 \) representation. (Notation is \(|N, \ell, m\rangle\)) It is called a
1P state because it is the first \(P\)-state.

Using the notation defined above,

\[|1, 1, \pm 1\rangle = a_{\pm}^\dagger |0\rangle\]

First, we show that \(|1, 1, 1\rangle\) cannot be raised:

\[L_+ |1, 1, 1\rangle = \hbar \sqrt{2}(a_x^+ a_z + a_z^+ a_-)a_+^\dagger |0\rangle = 0\]

Then by lowering the state,

\[L_- |1, 1, 1\rangle = \hbar \sqrt{2}(a_x^+ a_z + a_z^+ a_+)a_+^\dagger |0\rangle = \hbar \sqrt{2} |1, 1, 0\rangle\]

Lowering this state once more,

\[L_- |1, 1, 0\rangle = \hbar \sqrt{2}(a_x^+ a_z + a_z^+ a_+)a_+^\dagger |0\rangle = \hbar \sqrt{2} |1, 1, -1\rangle\]

Finally, this state cannot be lowered

\[L_- |1, 1, -1\rangle = \hbar \sqrt{2}(a_x^+ a_z + a_z^+ a_+)a_+^\dagger |0\rangle = 0\]

Therefore, they form the \(l = 1\) representation correctly.

(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.

We first rewrite the quadrupole operator in terms of creation and annihilation operators. Starting with

\[x_i = \sqrt{\frac{\hbar}{2m\omega}}(a_i + a_i^+)\]

we have

\[3z^2 - r^2 = 2z^2 - x^2 - y^2 = \frac{\hbar}{2m\omega} \left(2(a_z + a_z^+)^2 - (a_x + a_x^+)^2 - (a_y + a_y^+)^2\right)\]

\[= \frac{\hbar}{2m\omega} \left(2(a_z + a_z^+)^2 - \frac{1}{2}((a_- - a_+) + (a_-^+ a_+) + (a_-^+ a_+))\right)\]

Because we will take the expectation values of this operator, we are only interested in the pieces with one creation and one annihilation operators. The pieces with two creation or two annihilation operators do not give non-vanishing expectation values. Therefore, keeping only those terms,
we have

\[ 3z^2 - r^2 \sim \frac{\hbar}{m\omega} (a^+_z a^+_z + a^+_z a^-_z) - \frac{\hbar}{4m\omega} ((a_- - a_+)(a^+_z - a^+_z) + (a^+_z + a^+_z)(a_- - a_+)) - \frac{\hbar}{4m\omega} ((a_- + a_+)(a^+_z + a^+_z) + (a^+_z + a^+_z)(a_- + a_+)) \]

\[ = \frac{\hbar}{2m\omega} (2(a^+_z a^+_z + a^+_z a^-_z) - (a^-_a^+_a - a^+_a^-a + a^+_a^+_a + a^+_a^+_a)) = \frac{\hbar}{2m\omega} (2a^+_z a^-_z - (a^-_a^+_a + a^+_a^+_a)) \]

In the last step, we used the commutation relations to rewrite \(aa^+ = a^+a + 1\), and cancelled the constant pieces against each other. Then it is easy to work out the expectation values,

\[ \langle 1, 1, 1 | 3z^2 - r^2 | 1, 1, 1 \rangle = \langle 0 | a_+ \frac{\hbar}{m\omega} (2a^+_z a^-_z - (a^-_a^+_a + a^+_a^+_a)) a^+_a | 0 \rangle = -\frac{\hbar}{m\omega} \]

\[ \langle 1, 1, 0 | 3z^2 - r^2 | 1, 1, 0 \rangle = \langle 0 | a^- \frac{\hbar}{m\omega} (2a^+_z a^+_z - (a^+_a^+_a + a^+_a^+_a)) a^+_a | 0 \rangle = -2\frac{\hbar}{m\omega} \]

\[ \langle 1, 1, -1 | 3z^2 - r^2 | 1, 1, -1 \rangle = \langle 0 | a^- \frac{\hbar}{m\omega} (2a^+_z a^-_z - (a^+_a^+_a + a^+_a^+_a)) a^+_a | 0 \rangle = -\frac{\hbar}{m\omega} \]

The quadrupole moment operator here is a spherical tensor with rank \(k = 2, q = 0\). To see this result is consistent with the Wigner-Eckart theorem, we need the Clebsch-Gordan coefficients

\[
\text{Table[ClebschGordan}[[1, m], [2, 0], [1, m]], [m, -1, 1]]
\]

\[
\{ \frac{1}{\sqrt{10}}, -\sqrt{\frac{2}{5}}, \frac{1}{\sqrt{10}} \}
\]

The ratios among the expectation values are indeed the same as the ratios among the CG coefficients, \(1 : -2 : 1\). As an added note, a positive quadrupole moment \(\langle 3z^2 - r^2 \rangle > 0\) indicates a prolate form, while a negative quadrupole moment \(\langle 3z^2 - r^2 \rangle < 0\) indicates an oblated form.

(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).

From part (d) we can guess that the six states are composed of

\[ (a^+_z)^2 |0\rangle, \ (a^+_z)^2 |0\rangle, \ (a^+_z)^2 |0\rangle, \ a^+_z a^+_z |0\rangle, \ a^+_z a^+_z |0\rangle, \ a^+_z a^+_z |0\rangle \]
By looking at the $L_z$ eigenvalues, it is easy to identify
\[ |2, 2, 2\rangle = \frac{1}{\sqrt{2}} (a_+^*)^2 |0\rangle \]
\[ |2, 2, 1\rangle = a_+^* a_+^* |0\rangle \]
\[ |2, 2, -1\rangle = a_-^* a_-^* |0\rangle \]
\[ |2, 2, -2\rangle = \frac{1}{\sqrt{2}} (a_-^*)^2 |0\rangle \]

There are two states with $m = 0$: $(a_+^*)^2 |0\rangle$, $a_+^* a_+^* |0\rangle$. We can tell which linear combination belongs to the $l = 2$ representation by acting $L_-$ on $|2, 2, 1\rangle$,
\[ L_- |2, 2, 1\rangle = \hbar \sqrt{2} (a_+ a_z + a_+^* a_+) a_+^* |0\rangle \]
\[ = \hbar \sqrt{2} (a_+^* a_+^* + a_-^* a_-^*) |0\rangle = \hbar \sqrt{6} |2, 2, 0\rangle \]

Therefore we identify
\[ |2, 2, 0\rangle = \frac{1}{\sqrt{3}} (a_+^* a_+^* + a_-^* a_-^*) |0\rangle \]

which is properly normalized as it should be. The orthogonal combination is
\[ |2, 0, 0\rangle = \frac{1}{\sqrt{6}} (2a_+ a_+ - a_+^* a_-^*) |0\rangle \]

To verify that this state is indeed an $l = 0$ state, we can check
\[ L_+ |2, 0, 0\rangle = \hbar \sqrt{2} (a_+ a_z + a_+^* a_-) \frac{1}{\sqrt{6}} (2a_+ a_+ - a_+^* a_-^*) |0\rangle \]
\[ = \hbar \sqrt{2} \frac{1}{\sqrt{6}} (-a_+ a_+ + a_+^* a_-^* + 2a_- a_+^* |0\rangle = 0 \]

(h) How many possible states are there at the $N = 3, 4$ levels? What $\ell$ representations do they fall into?

For $N = 3$, it is clear that the state with the highest $L_z$ eigenvalue is $(a_+^*)^3 |0\rangle$ with $m = 3$. Hence it belongs to the $l = 3$ representation and has $2l + 1 = 7$ states. The only way to creat an $m = 2$ state is $a_z (a_+^*)^2 |0\rangle$, so there is no orthogonal $l = 2$ representation. However, there are two $m = 1$ states $(a_+^*)^2 a_+^* |0\rangle$ and $(a_+^*) a_+^* |0\rangle$, so there is an orthogonal $l = 1$ representation with 3 states. Finally there are two ways to make an $m = 0$ state, $(a_+^*)^3 |0\rangle$ and $a_+^* a_+^* a_+^* |0\rangle$, so there is not an additional $l = 0$ representation. Thus, there are 10 states in total.

Similarly, for $N = 4$, the highest representation must be $l = 4$ with 9 states. Learning from above, there are only three ways to make $m =$
0: \((a^+_\uparrow)^2(a^\downarrow\uparrow)^2|0\rangle\), \((a^+_\uparrow)^2a^\uparrow_\downarrow a^\downarrow_\uparrow|0\rangle\) and \((a^+_\uparrow)^4|0\rangle\), so there are three total representations. The only \(m = 3\) state is \(a^+_\uparrow(a^+_\downarrow)^3|0\rangle\), so there is no \(l = 3\); there are two \(m = 2\) states \((a^+_\uparrow)^3a^+_\downarrow|0\rangle\) and \(a^+_\uparrow(a^+_\downarrow)^2|0\rangle\), so there is an \(l = 2\) representation with 5 states. The final representation must be \(l = 0\) with 1 state. This gives 15 states total.

(i) What can you say about general \(N\)?

We note that the creation operators are linear combinations of \(\vec{x}\) and \(\vec{p}\) an hence parity odd. Therefore, if \(N = \text{even}\) states have even parity, and hence can only have even \(l\), while \(N = \text{odd}\) states have odd parity, and hence odd \(l\). In general, \(N = \text{even}\) states have \(l = 0, 2, 4, ..., N\), while \(N = \text{odd}\) states have \(l = 1, 3, 5, ..., N\). It can be verified by looking at the number of states (we will prove parity below).

The number of states at level \(N\) is the number of ways to make \(N\) selections of three objects \(a^+_\uparrow\), \(a^+_\downarrow\), and \(a^\downarrow_\downarrow\) with replacement. We may use the multiset \(3H^2 = N + 2\ C_N = (N + 2)(N + 1)/2\). For even \(N = 2k\), it is \((k + 1)(2k + 1)\).

Each \(l = 2j\) contributes \(2l + 1 = 4j + 1\) states, and the total is

\[
\sum_{j=0}^{k} (4j + 1) = 2k(k + 1) + (k + 1) = (k + 1)(2k + 1)
\]

For odd \(N = 2k - 1\), the number of states is \(k(2k + 1)\). Each \(l = 2j - 1\) contributes \(2l + 1 = 4j - 1\) states and the total is

\[
\sum_{j=1}^{k} (4j - 1) = 2k(k + 1) - k = k(2k + 1)
\]

(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 \(\Pi \vec{x} \Pi^+ = -\vec{x}\) and \(\Pi \vec{p} \Pi^+ = -\vec{p}\).

Recognizing that \(\vec{a}^+ \cdot \vec{a} = N\) is Hermitian, i.e.,

\[
(\vec{a}^+ \cdot \vec{a})^+ = (\vec{a})^+(\vec{a}^+)^+ = \vec{a}^+ \cdot \vec{a}
\]

we may use the Baker-Hausdorff formula to evaluate the expression:

\[
\Pi \vec{x} \Pi^+ = e^{i\pi N} \sqrt{\frac{\hbar}{2m\omega}}(\vec{a} + \vec{a}^+) \cdot e^{-i\pi N}
\]

\[
= \sqrt{\frac{\hbar}{2m\omega}} \sum_m \frac{(i\pi)^m}{m!} [N, [N, [N, ... [N, \vec{a} + \vec{a}^+] ...]]]\]

Noting that \([N, a] = -a\) and \([N, a^+] = a^+\), we may collapse this result
and separate even and odd terms:

\[
\Pi \vec{x} \Pi^+ = \sqrt{\frac{\hbar}{2m\omega}} \sum_m \frac{(i\pi)^m}{m!} ((-1)^m \vec{a} + \vec{a}^+) \\
= \sqrt{\frac{\hbar}{2m\omega}} \left( (\vec{a} + \vec{a}^+) \cos \pi + (-\vec{a} + \vec{a}^+) \sin \pi \right) = -\vec{x}
\]

\[
\Pi \vec{p} \Pi^+ = -\vec{p}
\]

follows immediately with

\[
\vec{x} \rightarrow \vec{p} = -i \sqrt{\frac{\hbar m\omega}{2}}(\vec{a} - \vec{a}^+)
\]

since only the odd term changes sign.

(k) Show that \( \Pi = (-1)^N \)

The computation is easy:

\[
\Pi |N, l, m \rangle = e^{i\pi \vec{a}^+ \cdot \vec{a}} |N, l, m \rangle \rightarrow \Pi = e^{i\pi N} = (e^{i\pi})^N = (-1)^N
\]

(l) Without calculating it explicitly, show that there are no dipole transitions from the 2\(P\) state to the 1\(P\) state. As we will see in Chapter 11, this means, show that \( \langle 1P | \vec{r} | 2P \rangle = 0 \).

Considering the Wigner-Eckart theorem, a 2\(P\) → 1\(P\) transition is allowed since \( \Delta l = 0 \) and \( l \neq 0 \). However, we note that 2\(P\) and 1\(P\) are both parity-odd eigenstates (which belong to odd \(N\) levels, as we have proved). The dipole operator is parity-odd, so the amplitude of the transition is zero by parity conservation. A parity-odd operator can only connect states of opposite parity under conservation.

9.7.63 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

\[ \hat{H} = \frac{\hat{L}_x^2}{2 I_\perp} + \frac{\hat{L}_z^2}{2 I_\parallel} \]

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

\[ E_{\ell,m} = \frac{\hbar^2}{2 I_\perp} \left( \ell(\ell + 1) - m^2 \left( 1 - \frac{I_\perp}{I_\parallel} \right) \right), \quad \psi_{\ell,m} = Y_{\ell m}(\theta, \phi) \]

What are the possible values for \( \ell \) and \( m \)? What are the degeneracies?

We seek solutions to \( \hat{H}\psi = E\psi \). Note that

\[ \hat{L}_x^2 + \hat{L}_y^2 = \hat{L}_z^2 - \hat{L}_z^2 \]

which implies that

\[ \hat{H} = \frac{\hat{L}_z^2}{2 I_\perp} - \left( \frac{1}{2 I_\perp} - \frac{1}{2 I_\parallel} \right) \hat{L}_z^2 = \frac{1}{2 I_\perp} \left( \hat{L}_z^2 - \left( 1 - \frac{I_\perp}{I_\parallel} \right) \hat{L}_z^2 \right) \]

Now the spherical harmonics are the eigenfunctions of \( \hat{L}_z^2 \) and \( \hat{L}_z^2 \) where

\[ \hat{L}_z^2 Y_{\ell m}^m(\theta, \phi) = \hbar^2 \ell(\ell + 1) Y_{\ell m}^m(\theta, \phi), \quad \hat{L}_z Y_{\ell m}^m(\theta, \phi) = \hbar m Y_{\ell m}^m(\theta, \phi) \]

This implies that the energy eigenfunctions are \( \psi_{\ell,m} = Y_{\ell m}^m \), i.e.,

\[ \hat{H}\psi_{\ell,m} = E_{\ell,m} \psi_{\ell,m} \]

\[ E_{\ell,m} = \frac{\hbar^2}{2 I_\perp} \left( \ell(\ell + 1) - m^2 \left( 1 - \frac{I_\perp}{I_\parallel} \right) \right) \]

The degeneracy is as follows: if \( m \neq 0 \), then the two states \( Y_{\ell m}^m \) and \( Y_{\ell -m}^{-m} \) have the same energy.
At $t = 0$, the system is prepared in the state

$$\psi_{\ell,m}(t = 0) = \sqrt{\frac{3}{4\pi}} x \sqrt{\frac{3}{4\pi}} \sin \theta \cos \phi$$

(b) Show that the state is normalized.

Normalization corresponds to

$$\int d\Omega |\psi_{\ell,m}|^2 = 1$$

where

$$d\Omega = d(\cos \theta) d\phi = dud\phi \quad (u = \cos \theta)$$

Now

$$\int d\Omega |\psi_{\ell,m}|^2 = \int d(\cos \theta) d\phi \frac{3}{4\pi} \sin^2 \theta \cos^2 \phi$$

$$= \int d(\cos \theta) d\phi \frac{3}{4\pi} (1 - \cos^2 \theta) \cos \theta = \frac{3}{4\pi} \int_{-1}^{1} du (1 - u^2) \int_{0}^{2\pi} \cos^2 \phi d\phi$$

$$= \frac{3}{4\pi} \left[ u - \frac{u^3}{3} \right]_{-1}^{1} \pi = \frac{3}{4\pi} \frac{4}{3} \pi = 1$$

(c) Show that

$$\psi_{\ell,m}(t = 0) = \frac{1}{\sqrt{2}} \left( -Y_1^1(\theta, \phi) + Y_1^{-1}(\theta, \phi) \right)$$

Given

$$Y_1^{\pm 1}(\theta, \phi) = \mp \sqrt{\frac{3}{8\pi}} \left( \frac{x \pm iy}{r} \right)$$

we have

$$\frac{1}{\sqrt{2}} \left( -Y_1^1 + Y_1^{-1} \right) = \frac{1}{\sqrt{2}} \sqrt{\frac{3}{8\pi}} \left( \frac{x + iy}{r} + \frac{x - iy}{r} \right)$$

$$= \frac{1}{\sqrt{2}} \sqrt{\frac{3}{8\pi}} \frac{2x}{r} = \sqrt{\frac{3}{4\pi}} \frac{x}{r}$$

so that

$$\psi_{\ell,m}(t = 0) = \frac{1}{\sqrt{2}} \left( -Y_1^1(\theta, \phi) + Y_1^{-1}(\theta, \phi) \right)$$

NOTE: This is clearly normalized since it is a superposition of $Y_2^\ell$'s; $\psi = \sum c_{\ell m} Y_{\ell m}$ and $\sum |c_{\ell m}|^2 = 1$.

(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.

$$\psi_{\ell,m}(t = 0) = \frac{1}{\sqrt{2}} \left( -Y_1^1(\theta, \phi) + Y_1^{-1}(\theta, \phi) \right)$$
\[
\hat{H}\psi = \frac{1}{\sqrt{2}} \left( -\hat{H}Y_1^1(\theta, \phi) + \hat{H}Y_{-1}^1(\theta, \phi) \right) \\
= \frac{1}{\sqrt{2}} \left( -E_{1,1}Y_1^1(\theta, \phi) + E_{1,-1}Y_{-1}^1(\theta, \phi) \right)
\]

But \(E_{1,1} = E_{1,-1}\) since \(E\) is independent of \(m\). Therefore we have \(\hat{H}\psi = E_{1,1}\psi\); it is an eigenfunction of \(\hat{H}\).

Because \(\psi\) is a superposition of degenerate eigenfunctions it is also an eigenfunction.

(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?

The possible values of \(\hat{L}^2\) and \(\hat{L}_z\) are their eigenvalues \(\hbar^2\ell(\ell + 1)\) and \(\hbar m\) with \(\ell = 0, 1, 2, \ldots\) and \(m = -\ell, -\ell + 1, \ldots, \ell\) for each \(\ell\) value. The probabilities are the expansion coefficients in \(\psi = \sum c_{\ell m}Y_{\ell m}\) such that \(P_{\ell m} = |c_{\ell m}|^2\).

Here

\[
\ell = 1 \text{ with probability } = 1 \\
m = +1 \text{ or } m = -1 \text{ with probability } = 1/2 \text{ each}
\]

9.7.64 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 \(eB > 0\))

\[
H = \frac{\Pi_x^2 + \Pi_y^2}{2m}, \quad \Pi_i = p_i - \frac{e}{c}A_i
\]

(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 \(\omega\).

We expand the Hamiltonian in the symmetric gauge

\[
H = \frac{1}{2m} (\Pi_x^2 + \Pi_y^2) = \frac{1}{2m} \left( \left( p_x - \frac{e}{c}A_x \right)^2 + \left( p_y - \frac{e}{c}A_y \right)^2 \right) \\
= \frac{1}{2m} \left( \left( p_x + \frac{eB}{c^2} y \right)^2 + \left( p_y - \frac{eB}{c^2} x \right)^2 \right)
\]

\[
H = \frac{1}{2m} (p_x^2 + p_y^2) + \frac{e^2B^2}{8mc^2}(x^2 + y^2) + \frac{eB}{2mc}(yp_x - xp_y) \\
= \frac{1}{2m} (p_x^2 + p_y^2) + \frac{m\omega^2}{2} (x^2 + y^2) + \omega(y p_x - x p_y)
\]

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where $\omega = eB/2mc$. Using the standard oscillators

$$a_x = \sqrt{\frac{m\omega}{2\hbar}} \left( x + \frac{i}{m\omega} p_x \right) \quad , \quad a_y = \sqrt{\frac{m\omega}{2\hbar}} \left( y + \frac{i}{m\omega} p_y \right)$$

we can recast our coordinates in oscillators

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a_x^+ + a_x) \quad , \quad p_x = i \sqrt{\frac{\hbar m\omega}{2}} (a_x^+ - a_x)$$

$$y = \sqrt{\frac{\hbar}{2m\omega}} (a_y^+ + a_y) \quad , \quad p_y = i \sqrt{\frac{\hbar m\omega}{2}} (a_y^+ - a_y)$$

Substituting back into the Hamiltonian,

$$H = -\frac{\hbar \omega}{4} ((a_x^+)^2 - a_x^+ a_x - a_x a_x^+ + a_x^2 + (a_y^+)^2 - a_y^+ a_y - a_y a_y^+ + a_y^2)$$

$$+ \frac{\hbar \omega}{4} ((a_x^+)^2 + a_x^+ a_x + a_x a_x^+ + a_x^2 + (a_y^+)^2 + a_y^+ a_y + a_y a_y^+ + a_y^2)$$

$$+ \frac{i \hbar \omega}{2} (a_y^+ a_x^+ - a_y^+ a_x - a_y^+ a_x^+ - a_y a_x - a_y a_y^+ + a_x^+ a_y - a_x a_y^+ + a_x a_y)$$

$$= \frac{\hbar \omega}{2} (a_x^+ a_x + a_x a_x^+ + a_y^+ a_y + a_y a_y^+ + 2i(a^+ x a_y - a_y^+ a_x))$$

Using the commutation relation $[a, a^+] = 1$, we have

$$H = \hbar \omega (a_x^+ a_x + a_y^+ a_y + 1 + i(a^+ x a_y - a_y^+ a_x))$$

(b) Further define $\hat{a}_z = (\hat{a}_x + i\hat{a}_y)/2$ and $\hat{a}_z^\dagger = (\hat{a}_x - i\hat{a}_y)/2$ and then rewrite the Hamiltonian using them. General states are given in the form

$$|n, m\rangle = \frac{(\hat{a}_x^+)^n (\hat{a}_z^+)^m}{\sqrt{n! m!}} |0, 0\rangle$$

starting from the ground state where $\hat{a}_z |0, 0\rangle = \hat{a}_z |0, 0\rangle = 0$. Show that they are Hamiltonian eigenstates of energies $\hbar \omega (2n + 1)$.

We have

$$a_x = \frac{1}{\sqrt{2}} (a_z + a_z^\dagger) \quad , \quad a_y = \frac{1}{\sqrt{2}} (a_z - a_z^\dagger)$$

which gives

$$H = \frac{\hbar \omega}{2} (a_z^+ + a_z^\dagger)(a_z + a_z^\dagger) - \frac{\hbar \omega}{2i} (a_z^+ - a_z^\dagger)(a_z^\dagger + a_z^\dagger)$$

$$+ \hbar \omega + \hbar \omega (a_z^+ + a_z^\dagger)(a_z - a_z^\dagger) - \hbar \omega (a_z^+ + a_z^\dagger)(a_z^\dagger + a_z^\dagger)$$

$$= \hbar \omega (a_z^+ a_z + a_z^\dagger a_z) + \hbar \omega + \frac{\hbar \omega}{2} (a_z^+ a_z - a_z^\dagger a_z + a_z^\dagger a_z)$$

$$+ \frac{\hbar \omega}{2} (a_z^+ a_z + a_z^\dagger a_z - a_z^+ a_z - a_z^\dagger a_z)$$

$$= \hbar \omega (2a_z^+ a_z + 1)$$
Now applying this Hamiltonian to the presumed eigenstates, we have

\[ H |n, m\rangle = \hbar \omega (2n^2 + 1) \left( \frac{\hat{a}_z^+}{\sqrt{n!}} \right) \left( \frac{(\hat{a}_z^+)^m}{\sqrt{m!}} \right) |0, 0\rangle \]

We need to commute the \( a_z \) through the daggered operators to the right. Let us evaluate the commutation relations:

\[ [a_z, a^+_z] = \frac{1}{2} [a_x + ia_y, a^+_x + ia^+_y] = \frac{1}{2} (1 + 1) = 1 \]

\[ [a_z, a^+_z] = \frac{1}{2} [a_x + ia_y, a^+_x + ia^+_y] = \frac{1}{2} (1 - 1) = 0 \]

Then, \( [a_z, (a^+_z)^n] = n(a^+_z)^{n-1} \) and so

\[ H |n, m\rangle = \hbar \omega (2n + 1) |n, m\rangle \]

as desired.

(c) For an electron, what is the excitation energy when \( B = 100 \text{kG} \)?

For an electron, the Bohr magneton is

\[ \mu_B = \frac{e \hbar}{2m_e} = 5.79 \times 10^{-11} \text{MeV T}^{-1} \]

The excitation energy

\[ \Delta E = \frac{e \hbar B}{2m_e} = 1.16 \times 10^{-3} \text{eV} \]

for \( B = 100 \text{kG} = 10 \text{T} \). The corresponding thermal energy is

\[ \frac{\Delta E}{k} = \frac{1.16 \times 10^{-3} \text{eV}}{8.62 \times 10^{-5} \text{eV K}^{-1}} = 13.4 \text{K} \]

At temperatures below a few Kelvin, practically all electrons populate the ground states.

(d) Work out the wave function \( \langle x, y | 0, 0\rangle \) in position space.

We have the requirement

\[ a_z |0, 0\rangle = \frac{1}{\sqrt{2}} (a_x + ia_y) |0, 0\rangle \]

\[ = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{m \omega}{2\hbar}} \left( x + \frac{i}{m \omega} p_x \right) + i \sqrt{\frac{m \omega}{2\hbar}} \left( y + \frac{i}{m \omega} p_y \right) \right) |0, 0\rangle \]

\[ = \sqrt{\frac{m \omega}{4\hbar}} \left( x + iy + \frac{1}{m \omega} (ip_x - p_y) \right) |0, 0\rangle = 0 \]
which in the position representation is

\[
\sqrt{\frac{m\omega}{4\hbar}} \left( x + iy + \frac{1}{m\omega} (i(-i\hbar \partial_x - (-i\hbar \partial_y)) \right) \psi_{0,0} = 0
\]

Similarly, for the requirement \( a_{\bar{z}} |0,0\rangle = 0 \), we have

\[
\sqrt{\frac{m\omega}{4\hbar}} \left( x - iy + \frac{\hbar}{m\omega} (\partial_x + i\partial_y) \right) \psi_{0,0} = 0
\]

To make our lives easier, let us change coordinates from \((x,y)\) to \((z,\bar{z})\) where \( z = x + iy \) and \( \bar{z} = x - iy \). then,

\[
\partial = \frac{1}{2} (\partial_x - i\partial_y) \quad \text{and} \quad \bar{\partial} = \frac{1}{2} (\partial_x + i\partial_y)
\]

such that

\[
\partial z = \bar{\partial} \bar{z} = 1 \quad \text{and} \quad \partial \bar{z} = \bar{\partial} z = 0
\]

Our equations then become

\[
\sqrt{\frac{m\omega}{4\hbar}} \left( z + 2\frac{\hbar}{m\omega} \partial \right) \psi_{0,0} = 0
\]

\[
\sqrt{\frac{m\omega}{4\hbar}} \left( \bar{z} + 2\frac{\hbar}{m\omega} \bar{\partial} \right) \psi_{0,0} = 0
\]

which have the solution

\[
\psi_{0,0} \propto e^{-m\omega z \bar{z}/2\hbar} = e^{-m\omega(x^2+y^2)/2\hbar}
\]

(c) \(|0, m\rangle\) are all ground states. Show that their position-space wave functions are given by

\[
\psi_{0,m}(z, \bar{z}) = N z^m e^{-cB z \bar{z}/4\hbar}
\]

where \( z = x + iy \) and \( \bar{z} = x - iy \). Determine \( N \).

For \( n = 0 \) and \( m \neq 0 \), the first requirement is the same as above,

\[
a_z \psi_{0,m} = \sqrt{\frac{m\omega}{4\hbar}} \left( z + 2\frac{\hbar}{m\omega} \partial \right) \psi_{0,m} = 0
\]

and this is clearly met by the form of the given wavefunction. For the second requirement, we use the number operator:

\[
a_{\bar{z}}^+ a_z |0, m\rangle = m |0, m\rangle
\]
In the position representation,
\[
a^+_z = \frac{1}{\sqrt{2}}(a^+_x + ia^+_y) = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{eB}{4\hbar c}} (x - \frac{2c}{eB} \text{i}p_x) + i \sqrt{\frac{eB}{4\hbar c}} (y - \frac{2c}{eB} \text{i}p_y) \right)
\]
\[
= \sqrt{\frac{eB}{8\hbar c}} \left( x + iy - \frac{2c}{eB} (\text{i}p_x - p_y) \right) = \sqrt{\frac{eB}{8\hbar c}} \left( x + iy - \frac{2c}{eB} (\text{i}(-\text{i}h\partial_x) - \text{i}h\partial_y) \right)
\]
\[
= \sqrt{\frac{eB}{8\hbar c}} \left( x + iy - \frac{2\hbar c}{eB} (\partial_x + i\partial_y) \right) = \sqrt{\frac{eB}{8\hbar c}} \left( z - \frac{\hbar c}{eB} \bar{\partial} \right)
\]
where \( \omega \) has been substituted so as not to confuse the eigenvalue \( m \) with the mass \( m \). Then, our requirement is
\[
a^+_z a_z |0, m\rangle = m |0, m\rangle
\]
\[
\rightarrow \frac{eB}{8\hbar c} \left( z - \frac{4\hbar c}{eB} \bar{\partial} \right) \left( \bar{z} + \frac{4\hbar c}{eB} \partial \right) \psi_{0,m} = m \psi_{0,m}
\]
\[
\rightarrow \left( \frac{eB}{8\hbar c} z\bar{z} + \frac{1}{2} z\partial - \frac{1}{2} \bar{z}\bar{\partial} - \frac{1}{2} \frac{\hbar c}{eB} \partial \bar{\partial} \right) |0, m\rangle = m |0, m\rangle
\]
Applying the LHS operator to the given wavefunction, we find
\[
\frac{eB}{8\hbar c} z\bar{z} + \frac{1}{2} z \left( \frac{m}{z} - \frac{eB}{8\hbar c} \bar{z} \right) - \frac{1}{2} - \frac{1}{2} \bar{z} \left( -\frac{eB}{8\hbar c} z \right) - \frac{2\hbar c}{eB} \bar{\partial} \left( \frac{m}{z} - \frac{eB}{8\hbar c} \bar{z} \right)
\]
\[
= \frac{eB}{8\hbar c} z\bar{z} + \frac{m}{2} - \frac{eB}{8\hbar c} z\bar{z} - \frac{1}{2} + \frac{eB}{8\hbar c} z\bar{z} - 2\frac{\hbar c}{eB} \left( -\frac{eB}{4\hbar c} + \left( \frac{m}{z} - \frac{eB}{4\hbar c} \bar{z} \right) \left( -\frac{eB}{4\hbar c} \bar{z} \right) \right)
\]
\[
= \frac{m}{2} - \frac{1}{2} + \frac{eB}{8\hbar c} z\bar{z} + \frac{m}{2} - \frac{eB}{8\hbar c} z\bar{z}
\]
\[
= m
\]
\( \psi_{0,m} \) is indeed the wavefunction \( \langle z, \bar{z} | 0, m \rangle \).

Now let us find \( N \):
\[
\int |\psi_{0,m}|^2 dxdy = N^2 \int dxdy(x^2 + y^2)^m e^{-eN(x^2+y^2)/2\hbar c}
\]
\[
= N^2 \int_0^\infty (2\pi r dr) r^2 m e^{-eBr^2/2\hbar c} = 1
\]
\[
\rightarrow N = \left( \int_0^\infty (2\pi r dr) r^2 m e^{-eBr^2/2\hbar c} \right)^{-1/2}
\]
Computing

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\[
\text{Integrate}\left[2\pi r*r^2e^{r}\right.\left.\frac{-eB}{2hc}r^2\right],
\]
\[
\{r, 0, \infty\}, \text{Assumptions} \rightarrow \{m > 0, e > 0, B > 0, h > 0, c > 0\}\right)^{-1/2}
\]
\[
\frac{1}{\sqrt{\pi}} \sqrt{2^{1-m} \left(\frac{hc}{\bar{e}}\right)^{1-m}} \Gamma(1+m)
\]

We find
\[
N = \left(\frac{\pi m!}{eB}\right)^{-1/2}
\]

Another way to find the wave function is directly working out
\[
\frac{(a_\bar{z})^m}{\sqrt{m!}} |0, 0\rangle
\]

From the previous part,
\[
\psi_{0,0} \propto e^{-m\omega z^2/2h} = e^{-m\omega(x^2+y^2)/2h}
\]

The correct normalization is easily obtained by the Gaussian integral and we find
\[
\psi_{0,0} = \sqrt{\frac{eB}{2\pi hc}} e^{-eBz\bar{z}/4hc}
\]

The creation operator was worked out above,
\[
a_\bar{z}^+ = \sqrt{\frac{eB}{8hc}} \left(z - \frac{4hc}{eB}\bar{z}\right)
\]

When we use this operator multiple times, there is never a derivative with respect to \(z\), and hence \(\bar{\partial}\) acts directly on \(\psi_{0,0}\). Namely, \(\bar{\partial} = -eBz/4hc\) as long as it acts only on the ground state wave functions. therefore,
\[
a_\bar{z}^+ = \sqrt{\frac{eB}{8hc}} \left(z - \frac{4hc}{eB}\bar{z}\right) = \sqrt{\frac{eB}{2hc}} z
\]

Using the definition,
\[
\psi_{0,m} = \frac{(a_\bar{z}^+)^m}{\sqrt{m!}} \psi_{0,0} = \frac{1}{\sqrt{m!}} \left(\frac{eB}{2hc}\right)^{m/2} z^m \sqrt{\frac{eB}{2\pi hc}} e^{-eBz\bar{z}/4hc}
\]
\[
= \left(\frac{1}{m! \pi} \left(\frac{eB}{2hc}\right)^{m+1}\right)^{1/2} z^m e^{-eBz\bar{z}/4hc}
\]

which is exactly the same result.
(f) Plot the probability density of the wave function for $m = 0, 3, 10$ on the same scale (use ContourPlot or Plot3D in Mathematica).

Take $eB/2\hbar c = 1$. Then

$$\psi_{0,m} = (m!\pi)^{-1/2} z^m e^{-z^2/2}$$

Therefore,

ContourPlot[$(m!\pi)^{-1} z^m E^{1/2} / \{x \rightarrow \sqrt{x^2 + y^2}\} \{m = 0\}$,
{x, -4, 4}, {y, -4, 4}, PlotPoints -> 100, PlotRange -> {0, 1/\pi}];

ContourPlot[$(m!\pi)^{-1} z^m E^{1/2} / \{x \rightarrow \sqrt{x^2 + y^2}\} \{m = 3\}$,
{x, -4, 4}, {y, -4, 4}, PlotPoints -> 100];
\[ \text{ContourPlot}\left\{\frac{1}{mn} e^{x^2 - \frac{1}{y^2}} \rightarrow \{x \rightarrow \sqrt{x^2 + y^2}\} \rightarrow (m \rightarrow 10), \{(x, -4, 4), (y, -4, 4), \text{PlotPoints} \rightarrow 100)\right\}; \]

\[ \text{Plot3D}\left\{\frac{1}{mn} e^{x^2 - \frac{1}{y^2}} \rightarrow \{x \rightarrow \sqrt{x^2 + y^2}\} \rightarrow (m \rightarrow 0), \{(x, -4, 4), (y, -4, 4), \text{PlotPoints} \rightarrow 100, \text{PlotRange} \rightarrow [0, \frac{1}{m}]\right\}; \]

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(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 $R$.

The wave function forms a ring further and further away from the origin for larger and larger $n$. If the system has a finite radius $R$, the ring goes outside the system for too large $n$. This sets a maximum value on $n$, and hence there are only a finite number of ground states. To obtain the maximum $n$, we require that the peak of the probability density is less than $R$. 

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For this radius to be inside the system, we must have
\[ \frac{2n\hbar}{eB} < R^2 \]
and hence
\[ n < \frac{eBR^2}{2\hbar} \]
The number of ground states is therefore \( eBR^2/2\hbar \).

(h) Show that the coherent state \( e^{j\tilde{a}^+} |0,0\rangle \) represents a near-classical cyclotron motion in position space.

Expanding the state in the Schrödinger picture,

\[
|\psi_c; t\rangle = e^{-iHt/\hbar} |\psi_c\rangle = e^{-iHt/\hbar} e^{j\tilde{a}^+} |0,0\rangle = \left( \sum \frac{e^{-iHt/\hbar}(f\tilde{a}_z^+)^l}{l!} |0,0\rangle \right) = e^{-i\omega t} \left( \sum (e^{-i2\omega t})^l \frac{(f\tilde{a}_z^+)^l}{l!} |0,0\rangle \right) = e^{-i\omega t} e^{-i2\omega t} a_z^+ |0,0\rangle
\]

In the position representation

\[
a_z^+ = \sqrt{\frac{m\omega}{4\hbar}} \left( \tilde{z} - \frac{2h}{m\omega} \theta \right) = \frac{1}{2} k_0 \left( \tilde{z} - \frac{1}{k_0^2} \theta \right)
\]

\[
\langle z, \tilde{z}, 0, 0 \rangle = \frac{1}{\sqrt{\pi \hbar}} e^{-m\omega \tilde{z}^2/2\hbar} \rightarrow \sqrt{\frac{2k_0^2}{\pi}} e^{-k_0^2 \tilde{z}^2}
\]

so the wavefunction is

\[
\langle z, \tilde{z} | \psi_c; t \rangle \propto e^{-i\omega t} e^{k_0 f e^{-i2\omega t}(\tilde{z} - (1/k_0^2)\theta) \tilde{z}} e^{-k_0^2 \tilde{z}^2}
\]

Making the coordinate transformation \( \tilde{z} \rightarrow \xi/fk_0 \),

\[
\langle \xi, \tilde{\xi} | \psi_c; t \rangle \propto e^{-i\omega t} e^{\xi e^{-i2\omega t} e^{-|\xi|^2/f^2}}
\]
The position wavefunction is a 2D Gaussian profile whose center moves clockwise on a circular path, which is precisely cyclotron motion of frequency \( 2\omega = eB/mc \) for an electron. (The first factor in the wavefunction is a time-dependent global phase due to the zero-point energy). To see this explicitly, we plot with \( \omega = 1, f = 2 \) and \( \xi = x + iy \). (To see the output, run the command below; then select the whole cell of plots, and create an animation by selecting the menu items ”Cell → Animate selected graphics” or by punching Control-y):

```math
9.7.65 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 \( L = \frac{1}{2} m R^2 \dot{\theta}^2 \) and write down the canonical momentum \( p_\theta \) and the Hamiltonian.

Into the Lagrangian of a point particle

\[
L = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2)
\]

we substitute in \( x = R \cos \theta, y = R \sin \theta \). Because the particle is always at the radius \( R \), we have

\[
\dot{x} = -R \dot{\theta} \sin \theta, \quad \dot{y} = R \dot{\theta} \cos \theta
\]

and hence

\[
L = \frac{1}{2} m R^2 \dot{\theta}^2
\]

The canonical momentum is given by its definition,

\[
p_\theta = \frac{\partial L}{\partial \dot{\theta}} = m R^2 \dot{\theta}
\]

The Hamiltonian is

\[
H = p_\theta \dot{\theta} - L = p_\theta \frac{p_\theta^2}{m R^2} - \frac{1}{2} m R^2 \left( \frac{p_\theta^2}{m R^2} \right)^2 = \frac{p_\theta^2}{2m R^2}
\]

(b) Write down the Heisenberg equations of motion and solve them, (So far no representation was taken).
The Heisenberg equation of motion is
\[ i\hbar \frac{d}{dt}\theta = [\theta, H] = \left[ \theta, \frac{p_\theta^2}{2mR^2} \right] = i\hbar \frac{p_\theta}{mR^2} \to \frac{d}{dt}\theta = \frac{p_\theta}{mR^2} \]
\[ i\hbar \frac{d}{dt}p_\theta = [p_\theta, H] = \left[ p_\theta, \frac{p_\theta^2}{2mR^2} \right] = 0 \to \frac{d}{dt}p_\theta = 0 \]

The solution to the second equation is simply \( p_\theta(t) = p_\theta(0) \) is conserved, and hence
\[ \theta(t) = \theta(0) + \frac{p_\theta}{mR^2}t \]

(c) Write down the normalized position-space wave function \( \psi_k(\theta) = \langle \theta \mid k \rangle \) for the momentum eigenstates \( \hat{p}_\theta |k\rangle = \hbar k |k\rangle \) and show that only \( k = n \in \mathbb{Z} \) are allowed because of the requirement \( \psi(\theta + 2\pi) = \psi(\theta) \).

The position-space wave function is given by
\[ \langle \theta \mid p_\theta \mid k \rangle = \frac{\hbar}{i} \frac{\partial}{\partial \theta} \langle \theta \mid k \rangle = \hbar k \langle \theta \mid k \rangle \]
so that
\[ \psi(\theta) = \langle \theta \mid k \rangle = Ne^{ik\theta} \]

To normalize it, we require
\[ \int_{0}^{2\pi} |\psi(\theta)|^2 d\theta = 2\pi N^2 = 1 \]
so that \( N = 1/\sqrt{2\pi} \) and hence
\[ \psi(\theta) = \frac{1}{\sqrt{2\pi}} e^{ik\theta} \]

In order to satisfy \( \psi(\theta + 2\pi) = \psi(\theta) \) which implies that \( e^{2\pi ik} = 1 \) we must have \( k = n \) an integer.

(d) Show the orthonormality
\[ \langle n \mid m \rangle = \int_{0}^{2\pi} \psi^*_n \psi_m d\theta = \delta_{nm} \]
\[ \langle n \mid m \rangle = \int_{0}^{2\pi} \langle n \mid \theta \rangle \langle \theta \mid m \rangle d\theta = \frac{1}{2\pi} \int_{0}^{2\pi} e^{i(m-n)\theta} d\theta \]

When \( n = m \), the integrand = 1, and hence \( \langle n \mid n \rangle = 1 \) and is normalized. When \( n \neq m \), \( \langle n \mid m \rangle = 0 \) and we have orthogonality.
(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

$$(A_x, A_y) = \begin{cases} B(-y, x)/2 & r < d \\ Bd^2(-y, x)/2r^2 & r > d \end{cases}$$

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.

With the vector potential, there is an additional term in the Lagrangian

$$L_{\text{int}} = q\vec{A} \cdot \vec{v} = q(A_x \dot{x} + A_y \dot{y}) = q\frac{Bd^2}{2R^2}(qR\dot{\theta} \sin \theta + xR\dot{\theta} \cos \theta) = \frac{1}{2}qBd^2\dot{\theta}$$

Therefore, the total Lagrangian is

$$L = \frac{1}{2}mR^2\dot{\theta}^2 + \frac{1}{2}qBd^2\dot{\theta}$$

and hence the canonical momentum is modified to

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mR^2\dot{\theta} + \frac{1}{2}qBd^2$$

Using

$$\dot{\theta} = \frac{p_\theta - \frac{1}{2}qBd^2}{mR^2}$$

the Hamiltonian is therefore (after some algebra)

$$H = p_\theta \dot{\theta} - L = \frac{1}{mR^2} \left(p_\theta - \frac{1}{2}qBd^2\right)^2$$

The eigenvalues of the canonical momentum are still $p_\theta = n\hbar$ because of the periodicity requirement and hence the energy eigenvalues are

$$E_n = \frac{1}{2mR^2} \left(n\hbar - \frac{1}{2}qBd^2\right)^2$$

Even though the particle never sees the magnetic field, the energy eigenvalues are affected by the vector potential, another manifestation of the Aharonov-Bohm effect. Note also that the result depends only on the total magnetic flux

$$\frac{q\Phi}{2\hbar} = \frac{qB\pi d^2}{2\pi \hbar} \text{ modulo integers}$$
9.7.66 Density Operators Redux

(a) Find a valid density operator $\rho$ 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 $\rho$ we have $\langle O_q \rangle = Tr[\rho O_q]$. Your density operator should be a $2 \times 2$ matrix with trace equal to one and eigenvalues $0 \leq \lambda \leq 1$. Prove that $\rho$ you find does not correspond to a pure state and therefore cannot be represented by a state vector.

We have

$$S_x \leftrightarrow \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y \leftrightarrow \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z \leftrightarrow \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and note that each of these matrices already has a zero trace. Hence

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

clearly satisfies the requirements to be a valid density operator (trace one, eigenvalues both equal to 1/2, Hermitian) and achieves

$$Tr[\rho S_{x,y,z}] = \frac{1}{2} Tr[S_{x,y,z}] = 0$$

Hence, with this state

$$\langle S_x \rangle = \langle S_y \rangle = \langle S_z \rangle = 0$$

We also have

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

and thus $Tr[\rho^2] = 1/2$, which proves that our $\rho$ is a mixed state.

(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

$$|\Psi\rangle \mapsto |\Psi_i\rangle = \frac{P_i |\Psi\rangle}{\sqrt{\langle \Psi | P_i | \Psi \rangle}}$$

Use this result to show that in density operator notation $\rho = |\Psi\rangle \langle \Psi |$ maps to

$$\rho_i = \frac{P_i \rho P_i}{Tr[\rho P_i]}$$

Both $\rho$ and $|\Psi\rangle$ here represent the same initial state, so the final states are also the same regardless of whether we work in the state vector or
the density matrix representation. Thus, we can simply take the final state according to the projection postulate for state vectors and form the corresponding density operator:

\[
|\Psi_i\rangle \leftrightarrow |\Psi_i\rangle \langle \Psi_i| = \frac{P_i |\Psi\rangle}{\sqrt{\langle \Psi | P_i |\Psi\rangle}} \sqrt{\langle \Psi | P_i |\Psi\rangle} = \frac{P_i |\Psi\rangle \langle \Psi| P_i}{\langle \Psi | P_i |\Psi\rangle} = \frac{P_i \rho P_i}{\langle \Psi | P_i |\Psi\rangle}
\]

There are many ways to show the final step, that

\[
\langle \Psi | P_i |\Psi\rangle = Tr[\rho P_i]
\]

An easy way is to use the fact that \(\rho^2 = \rho\) since it represents a pure state:

\[
Tr[\rho P_i] = [\rho^2 P_i] = Tr[\rho P_i \rho] = Tr[|\Psi\rangle \langle \Psi| P_i |\Psi\rangle \langle \Psi|] = \langle \Psi | P_i |\Psi\rangle Tr[\rho] = \langle \Psi | P_i |\Psi\rangle
\]

One could also compute the trace in terms of a complete basis \(|k\rangle\):

\[
Tr[\rho P_i] = \sum_k \langle k | \rho P_i | k \rangle = \sum_k \langle k | \langle \Psi | P_i |\Psi\rangle | k \rangle = \sum_k \langle \Psi | P_i |\Psi\rangle \sum_k \langle k | \langle k | | k \rangle = \langle \Psi | P_i |\Psi\rangle
\]

9.7.67 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: \([L_x, L_y] - i\hbar L_z\).

We have \(\hat{L} = \vec{r} \times \vec{p}\), so

\[
L_z = \frac{\hbar}{i} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)
\]

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and similarly for the other components, cyclically permuting $x, y, z$. The first commutator is just hard work:

$$L_x L_y = -\hbar^2 \left( \frac{y \partial}{\partial z} - \frac{z \partial}{\partial y} \right) \left( \frac{z \partial}{\partial x} - \frac{x \partial}{\partial z} \right)$$

$$= -\hbar^2 \left( y \frac{\partial^2}{\partial x \partial z} - xy \frac{\partial^2}{\partial y \partial z} - z^2 \frac{\partial^2}{\partial y \partial x} + zx \frac{\partial^2}{\partial y \partial z} \right)$$

Similarly,

$$L_y L_x = -\hbar^2 \left( \frac{z \partial}{\partial x} - \frac{x \partial}{\partial z} \right) \left( \frac{y \partial}{\partial z} - \frac{z \partial}{\partial y} \right)$$

$$= -\hbar^2 \left( x \frac{\partial^2}{\partial y \partial z} - xy \frac{\partial^2}{\partial x \partial z} - z^2 \frac{\partial^2}{\partial x \partial y} + zx \frac{\partial^2}{\partial x \partial z} \right)$$

Therefore, since mixed partials are independent of order, we have

$$[L_x, L_y] = -i\hbar L_z$$

(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 $[L_z, L_{\pm}]$.

We need to consider $L_z L_{\pm}$ which is

$$L_{\pm} L_z - [L_{\pm}, L_z]$$

The require commutator is readily proved from the basic commutators, we get:

$$[L_{\pm}, L_z] = \hbar L_{\pm}$$

Thus we have

$$L_z L_{\pm} |\ell, m\rangle = (L_{\pm} L_z + \hbar L_z) |\ell, m\rangle$$

or since $L_z |\ell, m\rangle = m\hbar |\ell, m\rangle$ we have

$$L_z L_{\pm} |\ell, m\rangle = (m \pm 1) |\ell, m\rangle$$

Therefore, the state $L_{\pm} |\ell, m\rangle$ is also an eigenstate of $L_z$, but its eigenvalues is $(m \pm 1)\hbar$; this is what we mean by raising or lowering.

(c) A system is in state $\psi$, 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 $\langle L_z^2 \rangle$. HINT: express $L_x$ in terms of $L_{\pm}$.

We have

$$L_x = \frac{L_+ + L_-}{2}$$
If \( \psi \) is the \( m \) eigenstate of \( L_z \), \( L_x \) produces a mixture of \( m-1 \) and \( m+1 \) states, which are orthogonal to the \( m \) state. Hence, \( \langle L_x \rangle = 0 \). Similarly,

\[
L_x^2 = \left( \frac{L_+ + L_-}{2} \right)^2 = \frac{1}{4}(L_+^2 + L_-^2 + L_+ L_- + L_- L_+)
\]

The expectation value of the first two terms vanishes, leaving

\[
\langle L_x^2 \rangle = \frac{1}{4} \langle L_+ L_- + L_- L_+ \rangle
\]

Now

\[
L_+ L_- + L_- L_+ = 2(L_x^2 + L_y^2) = 2(L^2 - L_z^2)
\]

Therefore,

\[
\langle L_x^2 \rangle = \frac{1}{2} \langle L^2 - L_z^2 \rangle = \frac{\hbar^2}{2} \ell (\ell + 1) - m^2
\]

The last step can also be argued by symmetry. We have

\[
\langle L^2 - L_z^2 \rangle = \langle L_x^2 \rangle + \langle L_y^2 \rangle
\]

but we expect \( \langle L_x^2 \rangle = \langle L_y^2 \rangle \).

(d) Hence show that \( L_x \) and \( L_y \) satisfy a general form of the uncertainty principle:

\[
\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq -\frac{1}{4} \langle [A, B] \rangle
\]

Now \( \langle (\Delta A)^2 \rangle = \langle (A - \langle A \rangle)^2 \rangle \). Therefore, we have \( \langle (\Delta L_x)^2 \rangle = \langle L_x^2 \rangle \) and \( \langle (\Delta L_y)^2 \rangle = \langle L_y^2 \rangle \). Therefore,

\[
\langle (\Delta L_x)^2 \rangle \langle (\Delta L_y)^2 \rangle = \frac{\hbar^4}{4} (\ell(\ell + 1) - m^2)^2
\]

Since the maximum value of \( m \) is \( \ell \), we have

\[
\langle (\Delta L_x)^2 \rangle \langle (\Delta L_y)^2 \rangle \geq \frac{\hbar^4 \ell^2}{4}
\]

Now consider the general uncertainty relation:

\[
\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq -\frac{\langle [A, B] \rangle^2}{4}
\]

and the fact that \( \langle [L_x, L_y] \rangle = i\hbar \langle L_z \rangle = im \hbar^2 \). Then the RHS of the uncertainty relation is \( \hbar^4 m^4/4 \). However, we already proved that the LHS was \( \geq \hbar^4 \ell^2/4 \) and \( \ell \geq m \), so this is consistent with the uncertainty relation (which becomes an equality when \( m = \ell \)).

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9.7.68 Wave Function Normalizability

The time-independent Schrödinger 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.

Normalization requires

\[
\int |\psi|^2 \, dV = 1 = \int |R|^2 r^2 \, dr \int |Y|^2 \sin \theta \, d\theta \, d\phi
\]

If \( R \propto r^{-\alpha} \), the radial integral is

\[
\propto \int r^{2-2\alpha} \, dr
\]

This diverges at \( r = 0 \) if \( 2 - 2\alpha < -1 \) or \( \alpha > 3/2 \). Thus, there is no objection to divergent wavefunctions from the point of view of normalization, provided that the divergence is not too extreme.

Now consider the energy eigenvalue, which is

\[
\langle H \rangle = \int \psi^* H \psi \, dV
\]

Now,

\[
H\psi = \left( \frac{\hbar^2}{2m} \left( \frac{1}{r^2} (r^2 \psi)' - \frac{\ell(\ell + 1)}{r^2} \psi \right) + V\psi
\]

If \( \psi \propto r^{-\alpha} \), the term in the square brackets is

\[
\frac{[\alpha(\alpha - 1) - \ell(\ell + 1)]\psi}{r^2}
\]

This vanishes if \( \alpha = -\ell \), but otherwise causes a divergent energy if \( \alpha > 1/2 \).

Whatever happens with the first term, the term

\[
\int \psi^* V\psi \, dV
\]

causes divergence at \( r = 0 \) if \( 2 - \alpha - (\alpha + \beta) < -1 \) where we assumed that \( V \propto r^{-\beta} \). Therefore, again the energy diverges if \( \alpha > (3 - \beta)/2 \).
Recall that we had a choice of $\psi \propto r^\ell$ or $\psi \propto r^{-(\ell+1)}$ in the Hydrogen atom solution. The reason we reject the second one is not that it cannot be normalized (it can, at least for $\ell - 0$), but because it gives divergent energies, which are unphysical. Many books say that the fact that $\psi$ diverges at $r = 0$ is reason enough to reject it, but this problem shows that divergent wavefunctions are OK - it is just that $\psi \propto r^{-(\ell+1)}$ is too divergent.

9.7.69 Currents

The quantum flux density of probability is

$$\vec{j} = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi)$$

It is related to the probability density $\rho = |\psi|^2$ by $\nabla \cdot \vec{j} + \dot{\rho} = 0$.

(a) Consider the case where $\psi$ is a stationary state. Show that $\rho$ and $\vec{j}$ are then independent of time. Show that, in one spatial dimension, $\vec{j}$ is also independent of position.

If $\psi$ is a stationary state, then

$$\psi(t) = \psi(0)e^{-iE t/\hbar}$$

Therefore,

$$\rho(t) = |\psi(t)|^2 = |\psi(0)|^2 = \rho(0) \rightarrow \text{time-independent}$$

We also have

$$\vec{j} = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi)$$

$$= \frac{i\hbar}{2m} (\psi(0)\nabla \psi^*(0) - \psi^*(0)\nabla \psi(0)) \rightarrow \text{time-independent}$$

Finally, we have

$$\nabla \cdot \vec{j} + \dot{\rho} = 0 \rightarrow \frac{dj}{dx} + \dot{\rho} = 0$$

But $\dot{\rho} = 0$, so we have

$$\frac{dj}{dx} = 0 \rightarrow \text{position-independent}$$

(b) Consider a 3D plane wave $\psi = Ae^{i\vec{k} \cdot \vec{x}}$. What is $\vec{j}$ in this case? Give a physical interpretation.

For $\psi = Ae^{i\vec{k} \cdot \vec{x}}$ we have

$$\nabla \psi = i\vec{k} \psi \quad , \quad \nabla \psi^* = -i\vec{k} \psi^*$$

Therefore,

$$\vec{j} = \frac{i\hbar}{2m} (-i\vec{k}|\psi|^2 - i\vec{k}|\psi|^2) = \frac{\hbar \vec{k}}{m} \rho = \rho \vec{v} \rightarrow \text{the flux density of probability}$$
9.7.70 Pauli Matrices and the Bloch Vector

(a) Show that the Pauli operators

\[ \sigma_x = \frac{2}{\hbar} S_x, \quad \sigma_y = \frac{2}{\hbar} S_y, \quad \sigma_z = \frac{2}{\hbar} S_z \]

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.

We have

\[ \sigma_x \leftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y \leftrightarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

so clearly

\[ \sigma_i^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]

which establishes the \( i = j \) parts of the equation we are trying to prove. For \( i \neq j \), we note that \( Tr[\sigma_i \sigma_j] = Tr[\sigma_j \sigma_i] \) so we need only compute three matrix products:

\[ \sigma_x \sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \leftrightarrow i\sigma_z \]

\[ \sigma_z \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \leftrightarrow i\sigma_y \]

\[ \sigma_y \sigma_z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \leftrightarrow i\sigma_x \]

These are all clearly traceless, which completes the proof.

(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:

\[ \rho = \frac{1}{2} (I + \langle \sigma_x \rangle \sigma_x + \langle \sigma_y \rangle \sigma_y + \langle \sigma_z \rangle \sigma_z) \]

We first use the parameterization and the result of part (a) to obtain

\[ Tr[\rho^2] = \frac{1}{2} (1 + \langle \sigma_x \rangle^2 + \langle \sigma_y \rangle^2 + \langle \sigma_z \rangle^2) \]
Since this is equal to the purity, we conclude that the state is pure if and only if
\[
\langle \sigma_x \rangle^2 + \langle \sigma_y \rangle^2 + \langle \sigma_z \rangle^2 = 1
\]
Since
\[
|\vec{s}|^2 = (S_x)^2 + (S_y)^2 + (S_z)^2
\]
\[
= \frac{\hbar^2}{4} (\langle \sigma_x \rangle^2 + \langle \sigma_y \rangle^2 + \langle \sigma_z \rangle^2)
\]
we conclude that $|\vec{s}| = 1$ if and only if the density operator represents a pure state.
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?

We have

\[ H = T + V(x) = T + V_s(x) + V(x) - V_s(x) = H_0 + H' \]

where

\[ V_s(x) = \begin{cases} 0 & \text{for } 0 \leq x \leq L \\
\infty & \text{for } x < 0 \text{ and } x > L 
\end{cases} \]

and

\[ H_0 = T + V_s(x) \]

which we know how to solve and

\[ H' = \begin{cases} 
-V_0 \sin(\pi x/L) & \text{for } 0 \leq x \leq L \\
0 & \text{for } x < 0 \text{ and } x > L 
\end{cases} \]

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.
With stationary states

\[ \varphi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \]

we have the energy correction to first-order in the perturbation

\[
\Delta E_n = \int_{-\infty}^{\infty} dx \varphi_n(x) \Delta V(x) \varphi_n(x)
\]

\[
= -\frac{V_0}{L} \int_0^L dx \sin \frac{\pi x}{L} \sin^2 \frac{n\pi x}{L} = -\frac{2V_0}{L} \int_0^L dx \sin \frac{\pi x}{L} \left(1 - \cos \frac{2n\pi x}{L}\right)
\]

\[
= -\frac{V_0}{L} \left[ -\frac{L}{\pi} \cos \frac{\pi x}{L} \right]_0^L + \frac{V_0}{L} \int_0^L dx \sin \frac{\pi x}{L} \cos \frac{2n\pi x}{L}
\]

\[
= -\frac{2V_0}{\pi} + \frac{V_0}{2L} \left[ \int_0^L dx \sin \frac{(2n+1)\pi x}{L} - \int_0^L dx \sin \frac{(2n-1)\pi x}{L} \right]
\]

\[
= -\frac{2V_0}{\pi} + \frac{V_0}{2L} \left[ \frac{L}{(2n+1)\pi} \left[ \cos \frac{(2n+1)\pi x}{L} \right]_0^L - \frac{L}{(2n-1)\pi} \left[ \cos \frac{(2n-1)\pi x}{L} \right]_0^L \right]
\]

\[
= -\frac{2V_0}{\pi} + \frac{V_0}{2L} \left[ \frac{L}{(2n+1)\pi} (-2) - \frac{L}{(2n-1)\pi} (-2) \right]
\]

\[
= -\frac{2V_0}{\pi} + \frac{V_0}{2\pi} \left[ \frac{1}{(2n+1)} (-2) - \frac{1}{(2n-1)} (-2) \right] = -\frac{V_0}{\pi} \frac{8n^2}{4n^2 - 1}
\]

All shifts are negative and for large \( n \), they approach

\[
\Delta E_n = -\frac{2V_0}{\pi}
\]

independent of \( n \).

### 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.
We have the perturbation
\[ \hat{H}' = \frac{V_0}{a} x, \quad 0 \leq x \leq a \]

The unperturbed eigenfunctions and corresponding energies (unperturbed) for the first three states are:

\[ \psi^{(0)}_1 = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}, \quad E^{(0)}_1 = \frac{\pi^2 \hbar^2}{2ma^2} \]
\[ \psi^{(1)}_1 = \sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}, \quad E^{(0)}_2 = \frac{2\pi^2 \hbar^2}{m a^2} \]
\[ \psi^{(2)}_1 = \sqrt{\frac{2}{a}} \sin \frac{3\pi x}{a}, \quad E^{(0)}_3 = \frac{9\pi^2 \hbar^2}{2ma^2} \]

The 1\(^{\text{st}}\)-order energy corrections are then

\[ \left\langle \psi^{(0)}_1 | \hat{H}' | \psi^{(0)}_1 \right\rangle = 2 \frac{V_0}{a} \int_0^a x \sin^2 \frac{\pi x}{a} dx = \frac{V_0}{2} \]
\[ \left\langle \psi^{(0)}_2 | \hat{H}' | \psi^{(0)}_2 \right\rangle = 2 \frac{V_0}{a} \int_0^a x \sin^2 \frac{2\pi x}{a} dx = \frac{V_0}{2} \]
\[ \left\langle \psi^{(0)}_3 | \hat{H}' | \psi^{(0)}_3 \right\rangle = 2 \frac{V_0}{a} \int_0^a x \sin^2 \frac{3\pi x}{a} dx = \frac{V_0}{2} \]

Therefore, to 1\(^{\text{st}}\)-order, the perturbed energies are

\[ E_1 = \frac{\pi^2 \hbar^2}{2ma^2} + \frac{V_0}{2} \]
\[ E_2 = \frac{2\pi^2 \hbar^2}{ma^2} + \frac{V_0}{2} \]
\[ E_3 = \frac{9\pi^2 \hbar^2}{2ma^2} + \frac{V_0}{2} \]

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 \( \Delta V = \lambda \sin kx \), \( \lambda \ll 1 \). Find the corrected ground state.

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The zeroth order system is a harmonic oscillator with
\[ H_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 \]
\[ \hat{x} = x_0 (\hat{a}^+ + \hat{a}) , \quad x_0 = \sqrt{\frac{\hbar}{2m\omega}} \]
\[ \hat{H}_0 = \hbar\omega (\hat{a}^+ \hat{a} + 1/2) \rightarrow E_n^{(0)} = \hbar\omega (n + 1/2) \]
\[ H_0 |n\rangle = E_n^{(0)} |n\rangle \]
\[ \hat{a} |n\rangle = \sqrt{n} |n-1\rangle , \quad \hat{a}^+ |n\rangle = \sqrt{n+1} |n+1\rangle \]

The corrected ground state will be
\[ |0\rangle' = |0\rangle + \sum_{n=1}^{\infty} \frac{\langle n| \Delta V |0\rangle}{E_0^{(0)} - E_n^{(0)}} |n\rangle = |0\rangle - \frac{\lambda}{\hbar\omega} \sum_{n=1}^{\infty} \frac{\langle n| \sin kx |0\rangle}{n} |n\rangle \]

The relevant matrix element can be written as the imaginary part of
\[ \langle n| e^{ikx} |0\rangle = \langle n| e^{ik\sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^+ + \hat{a})} |0\rangle \]

Since
\[ [\hat{a}, \hat{a}^+] = 1 \]
we can make use of the identity
\[ e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-[\hat{A}, \hat{B}]/2} \]
and obtain
\[ \langle n| e^{ikx} |0\rangle = \langle n| e^{ik\sqrt{\frac{\hbar}{2m\omega}} \hat{a}^+} e^{ik\sqrt{\frac{\hbar}{2m\omega}} \hat{a}} |0\rangle e^{-\frac{\hbar k^2}{4m\omega}} \]
\[ = \langle n| e^{ik\sqrt{\frac{\hbar}{2m\omega}} \hat{a}^+} \sum_{j=0}^{\infty} \frac{(ik\sqrt{\frac{\hbar}{2m\omega}} \hat{a}^+)^j}{j!} |0\rangle e^{-\frac{\hbar k^2}{4m\omega}} = \langle n| e^{ik\sqrt{\frac{\hbar}{2m\omega}} \hat{a}^+} |0\rangle e^{-\frac{\hbar k^2}{4m\omega}} \]
\[ = \langle n| \sum_{j=0}^{\infty} \frac{(ik\sqrt{\frac{\hbar}{2m\omega}} \hat{a}^+)^j}{j!} |0\rangle e^{-\frac{\hbar k^2}{4m\omega}} = \langle n| \sum_{j=0}^{\infty} \frac{(ik\sqrt{\frac{\hbar}{2m\omega}})^j}{j!} \sqrt{j!} |j\rangle e^{-\frac{\hbar k^2}{4m\omega}} \]
\[ = \sum_{j=0}^{\infty} \frac{(ik\sqrt{\frac{\hbar}{2m\omega}})^j}{j!} \sqrt{j!} \langle n | j \rangle e^{-\frac{\hbar k^2}{4m\omega}} = \sum_{j=0}^{\infty} \frac{(ik\sqrt{\frac{\hbar}{2m\omega}})^j}{j!} \delta_{nj} e^{-\frac{\hbar k^2}{4m\omega}} \]
\[ = \frac{(ik\sqrt{\frac{\hbar}{2m\omega}})^n}{\sqrt{n!}} e^{-\frac{\hbar k^2}{4m\omega}} \]

Therefore,
\[ \langle n| \sin kx |0\rangle = \frac{(ik\sqrt{\frac{\hbar}{2m\omega}})^n}{\sqrt{n!}} e^{-\frac{\hbar k^2}{4m\omega}} (1 - (-1)^n) \]
and

\[
|0'\rangle = |0\rangle - \frac{\lambda}{\hbar \omega} \sum_{n=0}^{\infty} \left( \frac{i k \sqrt{\frac{\hbar}{2m\omega}}}{in\sqrt{n!}} \right)^n e^{-\frac{\hbar k^2}{4m\omega}} |n\rangle
\]

\[
= |0\rangle - \frac{\lambda}{\hbar \omega} \sum_{q=0}^{\infty} \frac{(-1)^{2q+1} \left( k \sqrt{\frac{\hbar}{2m\omega}} \right)^{2q+1}}{(2q+1)\sqrt{(2q+1)!}} e^{-\frac{\hbar k^2}{4m\omega}} |2q+1\rangle
\]

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.

The energy and eigenfunction of the ground state of the unperturbed infinite well are

\[
\psi_1^{(0)} = \sqrt{\frac{1}{3a}} \cos \frac{\pi x}{6a}, \quad E_1^{(0)} = \frac{\pi^2 \hbar^2}{72ma^2}
\]

The 1st order energy correction is

\[
E^{(1)} = \left< \psi_1^{(0)} \middle| V(x) \middle| \psi_1^{(0)} \right> = \int_{-a}^{a} V_0 \left< \psi_1^{(0)} \right|^2 dx
\]

\[
= 2V_0 \int_{0}^{a} \frac{1}{3a} \cos^2 \frac{\pi x}{6a} dx = V_0 \left( \frac{1}{3} + \frac{\sqrt{3}}{2\pi} \right)
\]
Therefore the perturbed energy of the ground state to 1\textsuperscript{st} order is

\[ E = E^{(0)} + E^{(1)} = \frac{\pi^2 \hbar^2}{12ma^2} + V_0 \left( \frac{1}{3} + \frac{\sqrt{3}}{2\pi} \right) \]

10.9.5 Perturbing the 2-dimensional Infinite Square Well

Consider a particle in a 2-dimensional infinite square well given by

\[ V(x, y) = \begin{cases} 0 & \text{for } 0 \leq x \leq a \text{ and } 0 \leq y \leq a \\ \infty & \text{otherwise} \end{cases} \]

(a) What are the energy eigenvalues and eigenkets for the three lowest levels?

For the unperturbed system we have

\[ H = -\frac{\hbar^2}{2m} \nabla^2 + V(x) \quad , \quad E_{n_x n_y} = \frac{\pi^2 \hbar^2}{2ma^2} (n_x^2 + n_y^2) \]

\[ \psi_{n_x n_y}(x, y) = \frac{2}{a} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \quad , \quad n_x, n_y = 1, 2, \ldots \]

**Ground state:**

\[ n_x = n_y = 1 \quad , \quad E^{(0)}_{11} = \frac{\pi^2 \hbar^2}{ma^2} \]

\[ \psi^{(0)}_{11}(x, y) = \frac{2}{a} \sin \frac{\pi x}{a} \sin \frac{\pi y}{a} \quad , \quad \text{non-degenerate} \]

This is a non-degenerate level.

**1\textsuperscript{st} Excited state:**

\[ n_x = 1, n_y = 2 \quad , \quad E^{(0)}_{12} = \frac{5\pi^2 \hbar^2}{2ma^2} \]

\[ n_x = 2, n_y = 1 \quad , \quad E^{(0)}_{21} = \frac{5\pi^2 \hbar^2}{2ma^2} \]

\[ \psi^{(0)}_{12}(x, y) = \frac{2}{a} \sin \frac{\pi x}{a} \sin \frac{2\pi y}{a} \]

\[ \psi^{(0)}_{21}(x, y) = \frac{2}{a} \sin \frac{2\pi x}{a} \sin \frac{\pi y}{a} \]

This is a 2-fold degenerate level.

**2\textsuperscript{nd} Excited state:**

\[ n_x = n_y = 2 \quad , \quad E^{(0)}_{22} = \frac{4\pi^2 \hbar^2}{ma^2} \]

\[ \psi^{(0)}_{22}(x, y) = \frac{2}{a} \sin \frac{2\pi x}{a} \sin \frac{2\pi y}{a} \]

This is a non-degenerate level.

(b) We now add a perturbation given by

\[ V_1(x, y) = \begin{cases} \lambda xy & \text{for } 0 \leq x \leq a \text{ and } 0 \leq y \leq a \\ 0 & \text{otherwise} \end{cases} \]
Determine the first order energy shifts for the three lowest levels for $\lambda \ll 1$.

**First-order corrections**: the perturbation is

$$V_1(x, y) = \begin{cases} 
\lambda xy & \text{for } 0 \leq x \leq a \text{ and } 0 \leq y \leq a \\
0 & \text{otherwise}
\end{cases}$$

**Non-degenerate states**:

$$\langle 11 | V_1 | 11 \rangle = \int_0^a \int_0^a \frac{4}{\pi^2} \lambda xy \sin^2 \frac{\pi x}{a} \sin^2 \frac{\pi y}{a} dx dy = \frac{1}{4} \lambda a^2$$

$$\langle 22 | V_1 | 22 \rangle = \int_0^a \int_0^a \frac{4}{\pi^2} \lambda xy \sin^2 \frac{2\pi x}{a} \sin^2 \frac{2\pi y}{a} dx dy = \frac{1}{4} \lambda a^2$$

Therefore, to 1st order:

$$E_{11} = \frac{\pi^2 \hbar^2}{2ma^2} + \frac{1}{4} \lambda a^2$$

$$E_{22} = \frac{4 \pi^2 \hbar^2}{2ma^2} + \frac{1}{4} \lambda a^2$$

**Degenerate states**: we must diagonalize a $2 \times 2$ matrix. We have

$$\langle 12 | V_1 | 12 \rangle = \int_0^a \int_0^a \frac{4}{\pi^2} \lambda xy \sin^2 \frac{\pi x}{a} \sin^2 \frac{2\pi y}{a} dx dy = \frac{1}{4} \lambda a^2 = \langle 22 | V_1 | 22 \rangle$$

$$\langle 12 | V_1 | 21 \rangle = \int_0^a \int_0^a \frac{4}{\pi^2} \lambda xy \sin \frac{2\pi x}{a} \sin \frac{\pi y}{a} \sin \frac{\pi x}{a} \sin \frac{2\pi y}{a} dx dy = \frac{256}{81 \pi^2} \lambda a^2 = \langle 21 | V_1 | 12 \rangle$$

Therefore, the degenerate submatrix (to be diagonalized) is

$$\begin{pmatrix}
\frac{1}{4\pi^2} \lambda a^2 & \frac{1024}{81} \\
\frac{1024}{81} & \frac{81}{\pi^4}
\end{pmatrix}$$

This has eigenvalues

$$E_{\pm} = \frac{\lambda a^2}{4\pi^4} \left( \pi^4 \pm \frac{1024}{81} \right) = \begin{cases}
0.28 \lambda a^2 \\
0.22 \lambda a^2
\end{cases}$$

(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.

Therefore, the perturbed energy levels look like:
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.

(a) In the small angle approximation find the quantum mechanical energy levels of the system.

We take the equilibrium position of the point mass as the zero point of the potential energy. For the small angle approximation, the potential energy of the system is

$$V = mg\ell(1 - \cos \theta) \approx \frac{1}{2} mg\ell \theta^2$$

and the Hamiltonian is

$$H = \frac{1}{2} m\ell^2 \dot{\theta}^2 + \frac{1}{2} mg\ell \theta^2$$

which corresponds to a 1-dimensional harmonic oscillator. Therefore, we have

$$E_n^{(0)} = \hbar \omega (n + 1/2) \quad , \quad \omega = \sqrt{\frac{g}{\ell}}$$

(b) Find the lowest order correction to the ground state energy resulting from the inaccuracy of the small angle approximation.

The perturbation Hamiltonian is

$$H' = mg\ell(1 - \cos \theta) - \frac{1}{2} mg\ell \theta^2 \approx -\frac{1}{24} mg\ell \theta^4 = -\frac{1}{24} \frac{mg}{\ell^3} x^4 \quad , \quad x = \ell \theta$$
Now the ground state wave function of the harmonic oscillator is
\[ \psi_0 = \sqrt{\frac{\alpha}{\pi^{1/2}}} e^{-\frac{1}{2} \alpha^2 x^2} \quad , \quad \alpha = \sqrt{\frac{m \omega}{\hbar}} \]

Therefore, the lowest order correction to the ground state energy is
\[ E_0^{(1)} = -\frac{1}{24} \frac{mg}{\ell^3} \langle 0 | x^4 | 0 \rangle = -\frac{1}{24} \frac{mg}{\ell^3} \int_{-\infty}^{\infty} x^4 e^{-\alpha^2 x^2} dx = -\frac{1}{32} \frac{\hbar^2}{m \ell^2} \]

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.

We did some of this work in problem 8.15.9. here we have
\[ \hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 x^2 \quad , \quad \hat{H}'(x) = \alpha \hat{x}^3 + \beta \hat{x}^4 \]

with
\[ \hat{x} = x_0 (\hat{a} + \hat{a}^+) \quad , \quad x_0 = \sqrt{\frac{\hbar}{2m \omega}} \]
\[ \hat{H}_0 = \hbar \omega (\hat{a}^+ \hat{a} + 1/2) \rightarrow E_n^{(0)} = \hbar \omega (n + 1/2) \]
\[ \hat{H}_0 | n \rangle = E_n^{(0)} | n \rangle \]

and
\[ \hat{a} | n \rangle = \sqrt{n} | n - 1 \rangle \quad , \quad \hat{a}^+ | n \rangle = \sqrt{n + 1} | n + 1 \rangle \]

We then have
\[ \langle n' | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m \omega}} (\langle n' | \hat{a} | n \rangle + \langle n' | \hat{a}^+ | n \rangle) = \sqrt{\frac{\hbar}{2m \omega}} (\sqrt{n} \delta_{n',n-1} + \sqrt{n + 1} \delta_{n',n+1}) \]

From this result we get
\[ \langle n' | \hat{x}^2 | n \rangle = \sum_m \langle n' | \hat{x} | m \rangle \langle m | \hat{x} | n \rangle = \frac{\hbar}{2m \omega} \sum_m (\sqrt{m} \delta_{n',m-1} + \sqrt{m + 1} \delta_{n',m+1}) (\sqrt{n} \delta_{m,n-1} + \sqrt{n + 1} \delta_{m,n+1}) \]
\[ = \frac{\hbar}{2m \omega} (\sqrt{n(n-1)} \delta_{n',n-2} + \sqrt{(n+1)(n+2)} \delta_{n',n+2} + (2n + 1) \delta_{n',n}) \]

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and

\[ \langle n' | \hat{x}^3 | n \rangle = \sum_m \langle n' | \hat{x}^2 | m \rangle \langle m | \hat{x} | n \rangle \]

\[ = \left( \frac{\hbar}{2m\omega} \right)^{3/2} \sum_m \left( \frac{\sqrt{m(m-1)}\delta_{n',m-2}}{\sqrt{(m+1)(m+2)}\delta_{n',m+2} + (2m+1)\delta_{n',m}} \right) \times \left( \sqrt{n} + \sqrt{n+1} \delta_{m,n+1} \right) \]

\[ = \left( \frac{\hbar}{2m\omega} \right)^{3/2} \left( \frac{\sqrt{n(n-1)(n-2)}\delta_{n',n-3} + 3n\sqrt{n}\delta_{n',n-1}}{\sqrt{(n+1)(n+2)}\delta_{n',n+1} + \sqrt{(n+1)(n+2)(n+3)}\delta_{n',n+3}} \right) \]

and

\[ \langle n' | \hat{x}^4 | n \rangle = \sum_m \langle n' | \hat{x}^2 | m \rangle \langle m | \hat{x}^2 | n \rangle \]

\[ = \left( \frac{\hbar}{2m\omega} \right)^2 \sum_m \left( \frac{\sqrt{m(m-1)}\delta_{n',m-2}}{\sqrt{(m+1)(m+2)}\delta_{n',m+2} + (2m+1)\delta_{n',m}} \right) \times \left( \frac{\sqrt{n(n-1)}\delta_{m,n-2}}{\sqrt{(n+1)(n+2)}\delta_{m,n+2} + (2n+1)\delta_{m,n}} \right) \]

\[ = \left( \frac{\hbar}{2m\omega} \right)^2 \left( \frac{\sqrt{n(n-1)(n-2)(n-3)}\delta_{n',n-4} + 2(2n-1)\sqrt{n(n-1)}\delta_{n',n-2}}{\sqrt{(n+1)(n+2)(n+3)(n+4)}\delta_{n',n+2}} \right) \]

Using these matrix elements, we get

\begin{align*}
E_{n}^{(1)} & = \langle n | \hat{H} | n \rangle = \alpha \langle n | \hat{x}^3 | n \rangle + \beta \langle n | \hat{x}^4 | n \rangle = \beta \langle n | \hat{x}^4 | n \rangle \\
& = 3(2n^2 + 2n + 1)\beta \left( \frac{\hbar}{2m\omega} \right)^2 \\
\end{align*}

so that to 1st-order

\[ E_n = \hbar\omega(n + 1/2) + 3(2n^2 + 2n + 1)\beta \left( \frac{\hbar}{2m\omega} \right)^2 \]

(b) Evaluate all the required matrix elements of \( x^3 \) and \( x^4 \) needed to determine the wave function of the \( n^{th} \) state perturbed to 1st-order.

The state vector to 1st-order is

\[ |N\rangle = |n\rangle + \sum_{m \neq n} \frac{\langle m | \hat{H} | n \rangle}{E_n^{(0)} - E_m^{(0)}} |m\rangle = |n\rangle + \frac{\hbar}{\Delta E_n} \sum_{m \neq n} \frac{\langle m | \hat{H} | n \rangle}{n-m} |m\rangle \]

\[ = |n\rangle + a_{n-4} |n-4\rangle + a_{n-3} |n-3\rangle + a_{n-2} |n-2\rangle + a_{n-1} |n-1\rangle + a_{n+1} |n+1\rangle + a_{n+2} |n+2\rangle + a_{n+3} |n+3\rangle + a_{n+4} |n+4\rangle \]

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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

$$T = E - mc^2 = \sqrt{m^2 c^4 + p^2 c^2} - mc^2$$

(a) Determine the lowest order correction to the kinetic energy (a $p^4$ term).

We have

$$T = E - mc^2 = \sqrt{m^2 c^4 + p^2 c^2} - mc^2 = mc^2 \left( \sqrt{1 + \frac{p^2}{m^2 c^2}} - 1 \right)$$

$$\approx mc^2 \left( 1 + \frac{p^2}{2m^2 c^2} - \frac{p^4}{8m^4 c^4} + ... - 1 \right) = \frac{p^2}{2m} - \frac{p^4}{8m^3 c^2}$$

including only the largest correction.

Therefore,

$$H = T + V = \frac{p^2}{2m} - \frac{p^4}{8m^3 c^2} + \frac{1}{2} m \omega^2 x^2$$

$$= \left( \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \right) - \frac{p^4}{8m^3 c^2}$$

(b) Consider the correction to the kinetic energy as a perturbation and compute the relativistic correction to the ground state energy.

The unperturbed system is then

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \rightarrow a \ 1 \ - \ dimensional \ harmonic \ oscillator$$
where
\[ E_n^{(0)} = \hbar \omega (n + 1/2) \quad , \quad \hat{H}_0 \ket{n} = E_n^{(0)} \ket{n} \]
and the perturbation is
\[ H_1 = -\frac{p^4}{8m^3c^2} \]

The energy correction for the ground state is then
\[ E_0^{(1)} = \langle 0 \vert \hat{H}_1 \vert 0 \rangle = -\frac{1}{8m^3c^2} \langle 0 \vert \hat{p}^4 \vert 0 \rangle \]

where
\[ \hat{p} = ip_0 (\hat{a}^+ - \hat{a}) \quad , \quad p_0 = \sqrt{\frac{\hbar \omega}{2}} \]

Thus,
\[ E_0^{(1)} = -3\frac{\hbar^2 \omega^2}{32mc^2} \langle 0 \vert (\hat{a}^+ - \hat{a})^4 \vert 0 \rangle \]
\[ = -\frac{\hbar^2 \omega^2}{32mc^2} \langle 0 \vert (\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a}) \vert 0 \rangle \]
\[ = \frac{\hbar^2 \omega^2}{32mc^2} \langle 0 \vert \hat{a}^+(\hat{a}^+ - \hat{a}) (\hat{a}^+ - \hat{a}) \hat{a}^+ \vert 0 \rangle \]
\[ = \frac{\hbar^2 \omega^2}{32mc^2} \langle 1 \vert (\hat{a}^+ - \hat{a}) (\sqrt{6} \vert 3 \rangle - 3 \vert 1 \rangle \rangle \]
\[ = -3\frac{\hbar^2 \omega^2}{32mc^2} \langle 0 \vert (\hat{a}^+ - \hat{a}) (\hat{a}^+ - \hat{a}) (\hat{a}^+ - \hat{a}) (\hat{a}^+ - \hat{a}) \vert 0 \rangle \]

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 \( \hat{H}_0 = A\hat{S}_z^2 \).

We choose \( \hat{H}_0 = A\hat{S}_z^2 \). We have \( S = 1 \) and \( S_z = 0, \pm 1 \) in the unperturbed world (\( S_z \) basis)
\[
\begin{align*}
|+1\rangle & \rightarrow E_{+1}^{(0)} = Ah^2 \\
|0\rangle & \rightarrow E_0^{(0)} = 0 \\
|-1\rangle & \rightarrow E_{-1}^{(0)} = Ah^2
\end{align*}
\]

so that we have one non-degenerate level and a 2-fold degenerate level.
(b) Find the perturbed energy levels to first order.

We have
\[ \hat{V} = B(\hat{S}_z^2 - \hat{S}_y^2) = \frac{1}{4} B \left( (\hat{S}_+ \hat{S}_-) + (\hat{S}_+ \hat{S}_-) \right) = \frac{1}{2} B \left( \hat{S}_+^2 + \hat{S}_-^2 \right) \]

Therefore the \( V \) matrix is
\[
\begin{pmatrix}
0 & 2B\hbar^2 & 0 \\
2B\hbar^2 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]
with eigenvalues 0, \( \pm 2B\hbar^2 \). Thus, the new levels are non-degenerate.

(c) Solve the problem exactly by diagonalizing the Hamiltonian matrix in some basis. Compare to perturbation results.

The full \( H \) matrix is
\[
\begin{pmatrix}
A\hbar^2 & 2B\hbar^2 & 0 \\
2B\hbar^2 & A\hbar^2 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]
with eigenvalues 0, \( A\hbar^2 \pm 2B\hbar^2 \).

We can see that the exact eigenvalues agree with the 1st-order perturbation theory result. This means that there are no higher order correction in perturbation theory.

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
\[ \hat{H} = \hbar \omega_0 \hat{\sigma}_z + \frac{h\Omega}{2} \hat{\sigma}_x \]
where $\hbar \omega_0 = \mu_B B_z$ and $\hbar \Omega_0 = 2 \mu_B B_z$.

The Hamiltonian is

$$\hat{H} = -\vec{\mu} \cdot \vec{B} = (-2 \frac{\mu_B}{\hbar} \vec{S} \cdot \vec{B}) = \mu_B \sigma_x B_x + \mu_B \sigma_z B_z = \hbar \omega_0 \sigma_z + \frac{\hbar \Omega}{2} \sigma_x$$

where $\hbar \omega_0 = \mu_B B_z$ and $\frac{\hbar \Omega}{2} = \mu_B B_x$.

(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 $B_x / B_z$.

If $B_x = 0$, then $\hat{H}_0 = \hbar \omega_0 \sigma_z$ and for zeroth order we have

$$|\uparrow_z\rangle \Rightarrow E_{\uparrow}(0) = \hbar \omega_0$$
$$|\downarrow_z\rangle \Rightarrow E_{\downarrow}(0) = -\hbar \omega_0$$

Now we add a small field $|B_x|$ with $B_x \ll B_z$. Use perturbation theory with

$$\hat{H}_1 = \frac{\hbar \Omega}{2} \sigma_x$$

The first-order correction vanishes since

$$E_{\uparrow}(1) = \langle \uparrow | \hat{H}_1 | \uparrow \rangle = \frac{\hbar \Omega}{2} \langle \uparrow | \sigma_x | \uparrow \rangle = 0$$
$$E_{\downarrow}(1) = \langle \downarrow | \hat{H}_1 | \downarrow \rangle = \frac{\hbar \Omega}{2} \langle \downarrow | \sigma_x | \downarrow \rangle = 0$$

The second-order shift is

$$E_{\uparrow}^{(2)} = \frac{|\langle \uparrow | \hat{H}_1 | \uparrow \rangle|^2}{E_{\uparrow}^{(0)} - E_{\uparrow}^{(0)}} = \left( \frac{\hbar \Omega}{2} \right)^2 \frac{|\langle \uparrow | \sigma_x | \uparrow \rangle|^2}{2 \hbar \omega_0} = \frac{\hbar \omega_0}{2} \left( \frac{\Omega}{2 \omega_0} \right)^2 = \frac{\hbar \omega_0}{2} \left( \frac{B_x}{B_z} \right)^2$$
$$E_{\downarrow}^{(2)} = \frac{|\langle \downarrow | \hat{H}_1 | \downarrow \rangle|^2}{E_{\downarrow}^{(0)} - E_{\downarrow}^{(0)}} = \left( \frac{\hbar \Omega}{2} \right)^2 \frac{|\langle \downarrow | \sigma_x | \downarrow \rangle|^2}{-2 \hbar \omega_0} = -\frac{\hbar \omega_0}{2} \left( \frac{B_x}{B_z} \right)^2$$

Thus, to second-order we have

$$E_{\uparrow} = \hbar \omega_0 + \frac{\hbar \omega_0}{2} \left( \frac{B_x}{B_z} \right)^2 = \hbar \omega_0 \left( 1 + \frac{1}{2} \left( \frac{B_x}{B_z} \right)^2 \right)$$
$$E_{\downarrow} = -\hbar \omega_0 - \frac{\hbar \omega_0}{2} \left( \frac{B_x}{B_z} \right)^2 = -\hbar \omega_0 \left( 1 + \frac{1}{2} \left( \frac{B_x}{B_z} \right)^2 \right)$$

The lowest order corrections to the state vectors are:

$$|\uparrow_z\rangle \Rightarrow |\uparrow_z\rangle + |\downarrow_z\rangle \frac{|\langle \uparrow | \hat{H}_1 | \uparrow \rangle|^2}{E_{\uparrow}^{(0)} - E_{\downarrow}^{(0)}} = |\uparrow_z\rangle + \frac{1}{2} \frac{B_x}{B_z} |\downarrow_z\rangle$$
$$|\downarrow_z\rangle \Rightarrow |\downarrow_z\rangle - |\uparrow_z\rangle \frac{|\langle \downarrow | \hat{H}_1 | \downarrow \rangle|^2}{E_{\downarrow}^{(0)} - E_{\uparrow}^{(0)}} = |\downarrow_z\rangle - \frac{1}{2} \frac{B_x}{B_z} |\uparrow_z\rangle$$
(c) If $B_z = 0$, the eigenvectors are $|\uparrow_x\rangle$ and $|\downarrow_x\rangle$ with eigenvalues $\pm \hbar \Omega_0$ respectively. Now turn on a weak $z$ field with $B_z \ll B_x$. Use perturbation theory to find the new eigenvectors and eigenvalues to lowest order in $B_z/B_x$.

If $B_z = 0$, then

$$\hat{H}_0 = \frac{\hbar \Omega}{2} \sigma_x$$

and for zeroth order we have

$$|\uparrow_x\rangle \Rightarrow E^{(0)}_\uparrow = \frac{\hbar \Omega}{2}$$
$$|\downarrow_x\rangle \Rightarrow E^{(0)}_\downarrow = -\frac{\hbar \Omega}{2}$$

Now we add a small field $|B_z| \ll |B_x|$ and use perturbation theory with

$$\hat{H}_1 = \hbar \omega_0 \sigma_z$$

The first-order correction vanishes since

$$E^{(1)}_\uparrow = \langle \uparrow | \hat{H}_1 | \uparrow \rangle = \hbar \omega_0 \langle \uparrow | \sigma_z | \uparrow \rangle = 0$$
$$E^{(1)}_\downarrow = \langle \downarrow | \hat{H}_1 | \downarrow \rangle = \hbar \omega_0 \langle \downarrow | \sigma_z | \downarrow \rangle = 0$$

The second-order shift is

$$E^{(2)}_\uparrow = \frac{\langle \uparrow | \hat{H}_1 | \uparrow \rangle^2}{E^{(0)}_\uparrow - E^{(0)}_\downarrow} = (\hbar \omega_0)^2 \frac{\langle \uparrow | \sigma_z | \uparrow \rangle^2}{\hbar \Omega} = \frac{\hbar \Omega}{4} \left( \frac{2 \omega_0 \Omega}{\hbar} \right)^2 = \frac{\hbar \Omega}{4} \left( \frac{B_z}{B_x} \right)^2$$
$$E^{(2)}_\downarrow = \frac{\langle \downarrow | \hat{H}_1 | \downarrow \rangle^2}{E^{(0)}_\downarrow - E^{(0)}_\uparrow} = (\hbar \omega_0)^2 \frac{\langle \downarrow | \sigma_z | \downarrow \rangle^2}{\hbar \Omega} = -\frac{\hbar \Omega}{4} \left( \frac{B_z}{B_x} \right)^2$$

Thus, to second-order we have

$$E_\uparrow = \frac{\hbar \Omega}{2} + \frac{\hbar \Omega}{4} \left( \frac{B_z}{B_x} \right)^2 = \frac{\hbar \Omega}{2} \left( 1 + \frac{1}{2} \left( \frac{B_z}{B_x} \right)^2 \right)$$
$$E_\downarrow = -\frac{\hbar \Omega}{2} - \frac{\hbar \Omega}{4} \left( \frac{B_z}{B_x} \right)^2 = -\frac{\hbar \Omega}{2} \left( 1 + \frac{1}{2} \left( \frac{B_z}{B_x} \right)^2 \right)$$

(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.

For exact solutions we write the total Hamiltonian

$$\hat{H} = \hbar \omega_0 \sigma_z + \frac{\hbar \Omega}{2} \sigma_x$$

and as a matrix in the $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ basis

$$\hat{H} = \hbar \begin{bmatrix} \omega_0 & \frac{\Omega}{2} \\ \frac{\Omega}{2} & -\omega_0 \end{bmatrix}$$
The characteristic equation is

\[ \text{det}(\hat{H} - \hbar \lambda I) = \hbar^2 \left[ (\omega_0 - \lambda)(-\omega_0 - \lambda) - \frac{\Omega^2}{4} \right] = 0 \]

\[ \lambda_{\pm} = \pm \sqrt{\omega_0^2 + \frac{\Omega^2}{4}} \Rightarrow E_{\pm} = \pm \hbar \sqrt{\omega_0^2 + \frac{\Omega^2}{4}} \]

The eigenvectors are

\[ \hat{H} |\pm\rangle = E_{\pm} |\pm\rangle \]

|\pm\rangle = \left( \begin{array}{c} a_{\pm} \\ b_{\pm} \end{array} \right) \Rightarrow \omega_0 a_{\pm} + \frac{\Omega}{2} b_{\pm} = \lambda_{\pm} a_{\pm} \\
unnormalized: a_{\pm} = 1 \rightarrow b_{\pm} = \frac{\lambda_{\pm} - \omega_0}{\Omega/2} \\
|\pm\rangle = N_{\pm} \left[ \frac{\Omega}{2} |\uparrow_z\rangle + (\lambda_{\pm} - \omega_0) |\downarrow_z\rangle \right] \]

Let us now expand to lowest non-vanishing order in the small parameter

\[ \varepsilon = \frac{\Omega}{2\omega_0} = \frac{1}{2} \frac{B_z}{B_z} \]

We have

\[ E_{\pm} = \pm \hbar \sqrt{\omega_0^2 + \frac{\Omega^2}{4}} = \pm \hbar \omega_0 \sqrt{1 + \varepsilon^2} = \pm \hbar \omega_0 (1 + \frac{\varepsilon^2}{2}) = E_{\pm}^{(0)} + E_{\pm}^{(2)} \]

which agrees with part (b).

Expanding the eigenvectors we have

\[ |\pm\rangle = N_{\pm} \left[ \frac{\Omega}{2} |\uparrow_z\rangle + (\lambda_{\pm} - \omega_0) |\downarrow_z\rangle \right] \]

Now

\[ \lambda_{\pm} - \omega_0 = \omega_0 (\pm \sqrt{1 + \varepsilon^2} + 1) = \left( \begin{array}{c} \frac{\varepsilon^2}{2} \omega_0 \\
-2\omega_0 \end{array} \right) \]

so that

\[ |+\rangle = N_+ \left[ \frac{\Omega}{2} |\uparrow_z\rangle + (\lambda_+ - \omega_0) |\downarrow_z\rangle \right] = N_+ \left[ \frac{\Omega}{2} |\uparrow_z\rangle + \frac{\varepsilon^2}{2} \omega_0 |\downarrow_z\rangle \right] \]

\[ = N_+ \left[ |\uparrow_z\rangle - \frac{\Omega}{4\omega_0} |\downarrow_z\rangle \right] \]

\[ |-\rangle = N_- \left[ \frac{\Omega}{2} |\uparrow_z\rangle + (\lambda_- - \omega_0) |\downarrow_z\rangle \right] = N_- \left[ \frac{\Omega}{2} |\uparrow_z\rangle - 2\omega_0 |\downarrow_z\rangle \right] \]

\[ = N_- \left[ |\downarrow_z\rangle - \frac{\Omega}{4\omega_0} |\uparrow_z\rangle \right] \]

as before. A similar calculation shows that it agrees with part (c) also.

(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 $B_z \to \pm\infty$.

We have
This energy level diagram is known as an *avoided crossing*. In the absence of a $B_x$, the two energy levels would become degenerate at $B_x = 0$ (as shown above the dotted lines). Including $B_x$ the degeneracy is broken; the new eigenvectors are symmetric and antisymmetric combinations of $|↑⟩$ and $|↓⟩$.

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 $r_0 = 1.2 \times 10^{-13}\text{ cm}$ (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:

$$V(r) = \begin{cases} 
-\frac{Ze^2}{r} & \text{for } r > R \\
\frac{Ze^2}{R} \left( \frac{r}{2R^2} - \frac{1}{2} \right) & \text{for } r < R
\end{cases}$$

Draw a graph comparing this potential energy and the point nucleus potential energy.

For $r > R$, Gauss’ law says that the sphere of charge acts like a point charge at the center of the sphere. Therefore,

$$V(r) = -\frac{Ze^2}{r} \quad r > R$$
For $r < R$, Gauss’s law says that only the charge inside contributes. Therefore,

\[
\oint_{S} \varepsilon \cdot d \vec{A} = \varepsilon_r 4\pi r^2 = 4\pi (\text{charge inside}) = 4\pi Ze^2 \frac{r^3}{R^3}
\]

\[
\varepsilon_r = Ze^2 \frac{r}{R^3} \rightarrow \varphi = Ze^2 \frac{r^2}{2R^3} + C = \text{potential}
\]

\[
\rightarrow V(r) = Ze^2 \frac{r^2}{2R^3} + C = \text{potential energy}
\]

Now, continuity at $r - R$ gives

\[
Ze^2 \frac{R^2}{2R^3} + C = -Ze^2 \frac{r}{R} \rightarrow C = -\frac{3Ze^2}{2R}
\]

Therefore,

\[
V(r) = \begin{cases} 
-\frac{Ze^2}{R} & r > R \\
Ze^2 \frac{r^2}{2R^3} \left(\frac{r^3}{2\pi} - \frac{3}{2}\right) & r < R
\end{cases}
\]

The graph below chooses $Ze^2 = 1$ and $R = 1$ or

\[
V(r) = \begin{cases} 
-\frac{1}{r} & r > 1 \\
\frac{r^2}{\pi} - \frac{3}{2} & r < 1
\end{cases}
\]
(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 $\hat{H}_1$.

We then have

$$
\hat{H} = \frac{\hat{p}^2}{2m} + V(r) = \frac{\hat{p}^2}{2m} - \frac{Ze^2}{r} + \left(V(r) + \frac{Ze^2}{r}\right)
$$

$$
\hat{H}_0 = \frac{\hat{p}^2}{2m} - \frac{Ze^2}{r} \rightarrow \text{point charge at origin (hydrogen - like)}
$$

$$
\hat{H}_1 = V(r) + \frac{Ze^2}{r} = \begin{cases} 0 & r > R \\ \frac{Z e^2}{R} \left( \frac{r^2}{2R^2} - \frac{3}{2} \right) + \frac{Ze^2}{r} & r < R 
\end{cases}
$$

(c) Calculate (remember that $R \ll a_0 = \text{Bohr radius}$) the 1st-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?

The first-order correction to the ground state energy is

$$
E^{(1)}_0 = \int d^3r \psi_0^{\ast}(\vec{r}) \hat{H}_1(\vec{r}) \psi_0(\vec{r}),
$$

$$
\psi_0(\vec{r}) = \sqrt{\frac{\alpha}{\pi}} e^{-\alpha r}, \quad (\ell = 0), \quad \alpha = \frac{Z}{a_0}
$$

Now

$$
\frac{R}{a_0} = \frac{r_0}{a_0} A^{1/3} \approx 10^{-5} A^{1/3} \ll 1
$$

Therefore, we can approximate

$$
e^{-\alpha r/a_0} \approx 1 - \frac{\alpha r}{a_0} \text{ for } r < R \text{ (only region perturbation is nonzero)}
$$

so that we get

$$
E^{(1)}_0 = 4\alpha^3 \int_0^R r^2 dr \left( 1 - \frac{\alpha r}{a_0} + \left( \frac{2\alpha r}{a_0} \right)^2 \left( \frac{Ze^2}{R} \left( \frac{r^2}{2R^2} - \frac{3}{2} \right) + \frac{Ze^2}{r} \right) \right)
$$

$$
= 4\alpha^3 \left( \left( \frac{Ze^2}{R} \left( \frac{r^8}{16R^8} - \frac{3}{8} \right) + \frac{Ze^2R^2}{2} - \frac{2\alpha}{a_0} \left( \frac{Ze^2}{R} \left( \frac{r^6}{4R^6} - \frac{3}{10} \right) \right) \right) \right)
$$

$$
= 4\alpha^3 \left( \frac{1}{10} Ze^2 R^2 - \frac{\alpha}{12a_0} Ze^2 R^3 + \frac{3}{140} \left( \frac{2\alpha}{a_0} \right)^2 Ze^2 R^4 \right)
$$

$$
\approx \frac{2}{5} Ze^2 R^2 \alpha^3 = \frac{4}{5} \frac{Z^4 e^2}{2a_0} \left( \frac{R}{a_0} \right)^2
$$

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The effect compared to the ground states energy of hydrogen \((Z = 1)\) is

\[
\frac{|E^{(1)}_0|}{|E^{(0)}_0|} = \frac{4 \frac{e^2}{2\alpha_0} \left( \frac{R}{\alpha_0} \right)^2}{\frac{e^2}{2\alpha_0}} = \frac{4}{5} \left( \frac{R}{\alpha_0} \right)^2 \approx 10^{-10}
\]

This is the same size as the hyperfine splitting due to magnetic moment interactions.

### 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

\[
\{ |n\rangle \otimes |\downarrow\rangle, |n\rangle \otimes |\uparrow\rangle \}
\]

are energy eigenstates with eigenvalues \(E_{n,\downarrow} = n\hbar \omega\) and \(E_{n,\uparrow} = (n + 1)\hbar \omega\), respectively.

The basis set is

\[
\{ |n\rangle \otimes |\uparrow\rangle, |n\rangle \otimes |\downarrow\rangle \}, \quad n = 0, 1, 2, \ldots
\]

where

\[
\hat{H}_0 |n\rangle \otimes |\uparrow\rangle = \frac{\hbar \omega}{2} \hat{\sigma}_z |n\rangle \otimes |\uparrow\rangle + \hbar \omega \left( \hat{a}^+ \hat{a} + 1/2 \right) |n\rangle \otimes |\uparrow\rangle = \left( \hbar \omega (n + 1/2) + \frac{\hbar \omega}{2} \right) |n\rangle \otimes |\uparrow\rangle = \hbar \omega (n + 1/2) |n\rangle \otimes |\uparrow\rangle
\]

and

\[
\hat{H}_0 |n\rangle \otimes |\downarrow\rangle = \frac{\hbar \omega}{2} \hat{\sigma}_z |n\rangle \otimes |\downarrow\rangle + \frac{\hbar \omega}{2} \hat{\sigma}_z |n\rangle \otimes |\downarrow\rangle = \left( \hbar \omega (n + 1/2) - \frac{\hbar \omega}{2} \right) |n\rangle \otimes |\downarrow\rangle = \hbar \omega n |n\rangle \otimes |\downarrow\rangle
\]

so that \(\{ |n\rangle \otimes |\uparrow\rangle, |n\rangle \otimes |\downarrow\rangle \}, \quad n = 0, 1, 2, \ldots\) are eigenstates of \(\hat{H}_0\) with eigenvalues \(\{ n\hbar \omega (n + 1), \hbar \omega n \}\).

(b) The states associated with the ground-state energy and the first excited energy level are

\[
\{ |0\rangle \otimes |\downarrow\rangle, |1\rangle \otimes |\downarrow\rangle, |0\rangle \otimes |\uparrow\rangle \}
\]

What is(are) the ground state(s)? What is(are) the first excited state(s)? Note: two states are degenerate.

The ground state is

\[
|n = 0, \downarrow\rangle \Rightarrow E_{0,\downarrow} = 0
\]

The doubly degenerate first-excited states are

\[
|n = 1, \downarrow\rangle \Rightarrow E_{1,\downarrow} = \hbar \omega \quad |n = 0, \uparrow\rangle \Rightarrow E_{0,\uparrow} = \hbar \omega
\]

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(c) Now consider adding an interaction between the harmonic motion and the spin, described by the Hamiltonian

$$\hat{H}_1 = \frac{\hbar \Omega}{2} (\hat{a}\sigma_+ + \hat{a}^+\sigma_-)$$

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).

We add an interaction

$$\hat{H}_1 = \frac{\hbar \Omega}{2} (\hat{a}\sigma_+ + \hat{a}^+\sigma_-)$$

The matrix representation in the ground/first-excited-state subspace

\[ \{|n = 0, \downarrow\rangle, |n = 1, \downarrow\rangle, |n = 0, \uparrow\rangle\} \]

can be found using the results

\[
\begin{align*}
\hat{H}_1 |n = 0, \downarrow\rangle &= \frac{\hbar \Omega}{2} (\hat{a}\sigma_+ + \hat{a}^+\sigma_-) |n = 0, \downarrow\rangle = 0 \\
\hat{H}_1 |n = 1, \downarrow\rangle &= \frac{\hbar \Omega}{2} (\hat{a}\sigma_+ + \hat{a}^+\sigma_-) |n = 1, \downarrow\rangle = \frac{\hbar \Omega}{2} |n = 0, \uparrow\rangle \\
\hat{H}_1 |n = 0, \uparrow\rangle &= \frac{\hbar \Omega}{2} (\hat{a}\sigma_+ + \hat{a}^+\sigma_-) |n = 0, \uparrow\rangle = \frac{\hbar \Omega}{2} |n = 1, \downarrow\rangle
\end{align*}
\]

We have

$$H_1 = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & \frac{\hbar \Omega}{2} \\
0 & \frac{\hbar \Omega}{2} & 0
\end{pmatrix}$$

(d) Find the first order correction to the ground state and excited state energy eigenvalues for the subspace above.

To find the first-order corrections we have:

**Ground-state - nondegenerate:**

$$E^{(1)}_{0, \downarrow} = \langle n = 0, \downarrow | \hat{H}_1 | n = 0, \downarrow \rangle = 0$$

**First-excited-state - doubly degenerate:** Look at \( 2 \times 2 \) submatrix and find the eigenvalues from the characteristic equation

\[
\det \left( \begin{array}{cc}
-\lambda & \frac{\hbar \Omega}{2} \\
\frac{\hbar \Omega}{2} & -\lambda
\end{array} \right) = 0 \Rightarrow \lambda = \pm \frac{\hbar \Omega}{2}
\]

so that to first-order

$$E^{(1)}_{\pm} = \pm \frac{\hbar \Omega}{2}$$

The new eigenstates in the first-excited state subspace are

$$|\pm\rangle = \frac{1}{\sqrt{2}} (|n = 0, \uparrow\rangle \pm |n = 1, \downarrow\rangle)$$
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:

![Image of a spin-dependent trap](image)

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:

\[
\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega_{osc}^2 (\hat{z} - \Delta z/2)^2 \otimes \left| \uparrow_z \right> \left< \uparrow_z \right| + \frac{1}{2} m \omega_{osc}^2 (\hat{z} + \Delta z/2)^2 \otimes \left| \downarrow_z \right> \left< \downarrow_z \right|
\]

(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.

We have motion in a spin-dependent trap where the trap is correlated with internal states as shown in the figure above. The Hamiltonian that governs its dynamics is

\[
\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega_{osc}^2 (\hat{z} - \Delta z/2)^2 \otimes \left| \uparrow_z \right> \left< \uparrow_z \right| + \frac{1}{2} m \omega_{osc}^2 (\hat{z} + \Delta z/2)^2 \otimes \left| \downarrow_z \right> \left< \downarrow_z \right|
\]

In the absence of coupling (see Hamiltonian) between \( \left| \uparrow_z \right> \) and \( \left| \downarrow_z \right> \) there is a doubly degenerate spectrum. The energy levels are

\[
E_n = \hbar \omega (n + 1/2) , \quad n = 0, 1, 2, ....
\]

each with two distinct spin states \( \left| \uparrow_z \right> \) and \( \left| \downarrow_z \right> \). Thus, we have two orthogonal quantum states for each energy level

\[
|n\rangle_R \otimes \left| \uparrow_z \right>, \quad |n\rangle_L \otimes \left| \downarrow_z \right>
\]

where \( |n\rangle_R \) and \( |n\rangle_L \) are the Hermite-Gaussian wavefunctions centered in each well.
(b) A small, constant transverse field $B_x$ is now added with $|\mu_B B_x| \ll \hbar \omega_{osc}$. Qualitatively sketch how the energy plot in part (a) is modified.

We now turn on a small transverse magnetic field. The two states in each degenerate subspace are now coupled so that this perturbation will break the degeneracies. It might look like

\[
\begin{align*}
\frac{5}{2} \hbar \omega & \quad \rightarrow \quad z \\
\frac{3}{2} \hbar \omega & \quad \rightarrow \quad z \\
\frac{1}{2} \hbar \omega & \quad \rightarrow \quad z
\end{align*}
\]

This is not drawn to scale since the splittings are $\ll \hbar \omega$.

(c) Now calculate the perturbed energy levels for this system.

We now calculate using degenerate perturbation theory. Each energy level is doubly degenerate. Let

\[
|1\rangle = |n\rangle_L \otimes |\downarrow_z\rangle, \quad |2\rangle = |n\rangle_R \otimes |\uparrow_z\rangle
\]

The perturbation Hamiltonian is

\[
\hat{H}_1 = \mu_B B_x \hat{\sigma}_x = \frac{\hbar \Omega}{2} \hat{\sigma}_x
\]

We note that $\hat{H}_1$ does not couple the motional degrees of freedom - only the spin degrees of freedom, i.e., we really should write

\[
\hat{H}_1 = \frac{\hbar \Omega}{2} \hat{\sigma}_x \otimes \hat{I}_{motion}
\]

We must now diagonalize $\hat{H}_1$ in the $\{|1\rangle, |2\rangle\}$ basis. We have the matrix representation

\[
\hat{H}_1 = \begin{pmatrix}
\langle 1 | \hat{H}_1 | 1 \rangle & \langle 1 | \hat{H}_1 | 2 \rangle \\
\langle 2 | \hat{H}_1 | 1 \rangle & \langle 2 | \hat{H}_1 | 2 \rangle
\end{pmatrix}
\]
where

\[ (1) \hat{H}_1 |1\rangle = \langle \downarrow_z | \otimes L \langle n \mid \frac{\hbar \Omega}{2} \hat{\sigma}_x \otimes \hat{I}_{\text{motion}} \mid \downarrow_z \rangle |n\rangle_L \]

\[ = \frac{\hbar \Omega}{2} \langle \downarrow_z \mid \hat{\sigma}_x \rangle L \langle n \mid \hat{I}_{\text{motion}} |n\rangle_L = 0 \]

\[ (2) \hat{H}_1 |2\rangle = \langle \uparrow_z | \otimes R \langle n \mid \frac{\hbar \Omega}{2} \hat{\sigma}_x \otimes \hat{I}_{\text{motion}} \mid \uparrow_z \rangle |n\rangle_R \]

\[ = \frac{\hbar \Omega}{2} \langle \uparrow_z \mid \hat{\sigma}_x \rangle R \langle n \mid \hat{I}_{\text{motion}} |n\rangle_R = 0 \]

\[ (1) \hat{H}_1 |2\rangle = \langle \downarrow_z | \otimes L \langle n \mid \frac{\hbar \Omega}{2} \hat{\sigma}_x \otimes \hat{I}_{\text{motion}} \mid \uparrow_z \rangle |n\rangle_R \]

\[ = \frac{\hbar \Omega}{2} \langle \downarrow_z \mid \hat{\sigma}_x \rangle L \langle n \mid \hat{I}_{\text{motion}} |n\rangle_R = \frac{\hbar \Omega}{2} \langle n_L \mid n_R \rangle = (2) \hat{H}_1 |1\rangle^* \]

\[ (2) \hat{H}_1 |1\rangle = \frac{\hbar \Omega}{2} \langle n_L \mid n_R \rangle^* = \frac{\hbar \Omega}{2} \langle n_L \mid n_R \rangle \]

where the last step follows since the motion wavefunctions are real.

Thus,

\[ \hat{H}_1 = \left( \begin{array}{cc} \frac{\hbar \Omega}{2} \langle n_L \mid n_R \rangle & \frac{\hbar \Omega}{2} \langle n_L \mid n_R \rangle \\ \frac{\hbar \Omega}{2} \langle n_L \mid n_R \rangle & \frac{\hbar \Omega}{2} \langle n_L \mid n_R \rangle \end{array} \right) \]

as we would expect. The eigenvalues are

\[ E^{(1)}_{\pm} = \pm \frac{\hbar \Omega}{2} \langle n_L \mid n_R \rangle \]

where

\[ \langle n_L \mid n_R \rangle = \int_{-\infty}^{\infty} dz \varphi_n(z - \Delta z/2)(z + \Delta z/2) = \text{overlap of the wavefunctions} \]

Note: Unlike the spin in free space, here the splitting between the spin states depends on the spatial overlap of the two wavefunctions. This is known as tunneling splitting, as the particle must tunnel to the neighboring well in order to flip its spin.

(d) What are the new eigenstates in the ground-state doublet? For \( \Delta z \) macroscopic, these are sometimes called Schrodinger cat states. Explain why.

The eigenvectors are entangled states

\[ |\pm\rangle = \frac{1}{\sqrt{2}} (|1\rangle \pm |2\rangle) = \frac{1}{\sqrt{2}} (|n\rangle_L \otimes \downarrow_z \pm |n\rangle_R \otimes \uparrow_z) \]

which are the same as the Schrodinger cat states of the form

\[ |\pm\rangle = \frac{1}{\sqrt{2}} (|\text{decay}\rangle \otimes |\text{dead}\rangle \pm |\text{no decay}\rangle \otimes |\text{alive}\rangle) \]
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

$$\Delta V(x, y, z) = kxyz + \frac{k^2}{\hbar\omega} x^2 y^2 z^2$$

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!

We have $H = H_0 + \Delta V$ where

$$H_0 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + \frac{1}{2} m\omega^2(x^2 + y^2 + z^2)$$

gives the unperturbed world

$$|n_x, n_y, n_z\rangle \rightarrow E^{(0)}_{n_x n_y n_z} = \hbar\omega (n_x + n_y + n_z + 3/2)$$

and

$$\Delta V = kxyz + \frac{k^2}{\hbar\omega} x^2 y^2 z^2$$

First-order energy correction: From earlier problems we have

$$\langle n'| \hat{\chi} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left( \sqrt{n}\delta_{n', n-1} + \sqrt{n+1}\delta_{n', n+1} \right)$$

$$\langle n'| \hat{\chi}^2 | n \rangle = \frac{\hbar}{2m\omega} \left( \sqrt{n(n-1)}\delta_{n', n-2} + \sqrt{(n+1)(n+2)}\delta_{n', n+2} + (2n+1)\delta_{n', n} \right)$$

Therefore,

$$E^{(1)}_{n_x n_y n_z} = k \langle n_x, n_y, n_z | xyz | n_x, n_y, n_z \rangle + \frac{k^2}{\hbar\omega} \langle n_x, n_y, n_z | x^2 y^2 z^2 | n_x, n_y, n_z \rangle$$

$$= k \langle n_x | x | n_x \rangle \langle n_y | y | n_y \rangle \langle n_z | z | n_z \rangle + \frac{k^2}{\hbar\omega} \langle n_x | x^2 | n_x \rangle \langle n_y | y^2 | n_y \rangle \langle n_z | z^2 | n_z \rangle$$

$$= \frac{k^2}{\hbar\omega} \left( \frac{\hbar}{2m\omega} \right)^3 (2n_x + 1)(2n_y + 1)(2n_z + 1)$$

so that for the ground state

$$E^{(1)}_{000} = \frac{k^2}{\hbar\omega} \left( \frac{\hbar}{2m\omega} \right)^3 \rightarrow O(k^2)$$

which is 2nd-order in $k$

Second-order energy correction: We have

$$E^{(2)}_{000} = \sum_{n_x, n_y, n_z \neq 0} \frac{|\langle n_x, n_y, n_z | \Delta V | n_x, n_y, n_z \rangle|^2}{E^{(0)}_{000} - E_{n_x n_y n_z}}$$
Now the $xyz$ term $\to O(k^2)$ effect, but the $x^2y^2z^2$ term $\to O(k^4)$ effect, which we can neglect. Therefore,

$$E^{(2)}_{000} = k^2 \sum_{n_x,n_y,n_z \neq 0} \frac{|\langle n_x, n_y, n_z | xyz | 0, 0, 0 \rangle|^2}{3\hbar \omega/2 - \hbar \omega (n_x + n_y + n_z + 3/2)}$$

$$= -k^2 \sum_{n_x,n_y,n_z \neq 0} \frac{|\langle n_z | x | 0 \rangle \langle n_y | y | 0 \rangle \langle n_z | z | 0 \rangle|^2}{\hbar \omega (n_x + n_y + n_z)}$$

Now,

$$\langle n_x | x | 0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} (n_x | (\hat{a} + \hat{a}^+) | 0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \delta_{n_x,1}$$

Therefore,

$$E^{(2)}_{000} = -k^2 \sum_{n_x,n_y,n_z \neq 0} \frac{|\langle n_x | x | 0 \rangle \langle n_y | y | 0 \rangle \langle n_z | z | 0 \rangle|^2}{\hbar \omega (n_x + n_y + n_z)}$$

$$= -k^2 \left( \frac{\hbar}{2m\omega} \right)^3 \frac{1}{3\hbar \omega} = -\frac{1}{3} \left( \frac{\hbar}{2m\omega} \right)^3 \frac{k^2}{\hbar \omega}$$

and the energy shift to 2nd–order $(O(k^2))$ is

$$\Delta E = E^{(1)}_{000} + E^{(2)}_{000} = \frac{2}{3} \left( \frac{\hbar}{2m\omega} \right)^3 \frac{k^2}{\hbar \omega}$$

### 10.9.15 Another Perturbed Oscillator

Consider the system described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 \left( 1 - e^{-\alpha x^2} \right)$$

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

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

We have

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} (1 - e^{-\alpha x^2}) = H_0 + V$$

$$H_0 = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$$

$$V = \frac{m\omega^2}{2\alpha} (1 - e^{-\alpha x^2}) - \frac{m\omega^2}{2} x^2 = \frac{m\omega^2}{2} \left[ 1 - e^{-\alpha x^2} - \frac{1}{\alpha} x^2 \right]$$

The normalized unperturbed ground state energy eigenfunction of the unperturbed harmonic oscillator is

$$\varphi_0 = \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} e^{-\left( \frac{m\omega}{2\alpha} \right) x^2}$$
Thus, the first-order correction to the ground-state energy is

$$\langle \varphi_0 | V | \varphi_0 \rangle = \left( \frac{m\omega}{\pi \hbar} \right)^{1/2} \frac{m\omega^2}{2} \int_{-\infty}^{\infty} dx e^{-\left( \frac{m\omega}{\hbar} \right) x^2} \left[ \frac{1 - e^{-\alpha x^2}}{\alpha} - x^2 \right]$$

Now

$$\int_{0}^{\infty} x^\beta e^{-\lambda x^2} dx = \frac{1}{2} \Gamma\left( \frac{\alpha + 1}{2} \right)$$

$$\Gamma(x + 1) = x\Gamma(x), \quad \Gamma(1) = 1, \quad \Gamma(1/2) = \sqrt{\pi}$$

so that

$$\langle \varphi_0 | V | \varphi_0 \rangle = \left( \frac{m\omega}{\pi \hbar} \right)^{1/2} \frac{m\omega^2}{2} \int_{-\infty}^{\infty} dx e^{-\left( \frac{m\omega}{\hbar} \right) x^2} \left[ \frac{1 - e^{-\alpha x^2}}{\alpha} - x^2 \right]$$

$$= \left( \frac{m\omega}{\pi \hbar} \right)^{1/2} \frac{m\omega^2}{2} \left( \frac{1}{\alpha} \int_{-\infty}^{\infty} dx e^{-\left( \frac{m\omega}{\hbar} \right) x^2} - \frac{1}{\alpha} \int_{-\infty}^{\infty} dx e^{-\left( \frac{m\omega}{\hbar} + \alpha \right) x^2} - \int_{-\infty}^{\infty} dx x^2 e^{-\left( \frac{m\omega}{\hbar} \right) x^2} \right)$$

$$= \left( \frac{m\omega}{\pi \hbar} \right)^{1/2} \frac{m\omega^2}{2} \left( \frac{1}{\alpha} \frac{1}{\sqrt{\frac{m\omega}{\hbar}}} \Gamma(1/2) - \frac{1}{\alpha} \frac{1}{\sqrt{\frac{m\omega}{\hbar} + \alpha}} \Gamma(1/2) + \frac{1}{2} \frac{\Gamma(3/2)}{\left( \frac{m\omega}{\hbar} \right)^{3/2}} \right)$$

$$= \left( \frac{m\omega}{\pi \hbar} \right)^{1/2} \frac{m\omega^2}{2} \left( \frac{1}{1 + \frac{\alpha}{m\omega}} \right) = \frac{m\omega^2}{2\alpha} \left[ 1 - \frac{1}{\sqrt{1 + \frac{\alpha}{m\omega}}} \right] - \frac{\hbar \omega}{4}$$

Therefore the ground state energy is

$$E_0 = E_0^{(0)} + \langle \varphi_0 | V | \varphi_0 \rangle = \frac{\hbar \omega}{2} + \frac{m\omega^2}{2\alpha} \left[ 1 - \frac{1}{\sqrt{1 + \frac{\alpha}{m\omega}}} \right] - \frac{\hbar \omega}{4}$$

$$= \hbar \omega \left[ \frac{1}{4} + \frac{m\omega}{2\alpha} \left[ 1 - \frac{1}{\sqrt{1 + \frac{\alpha}{m\omega}}} \right] \right]$$

$$= \frac{1}{4} \hbar \omega \left[ 1 - \frac{1}{\sqrt{1 + \frac{\alpha}{m\omega}}} \right]$$

(2) Calculate an approximate value for the ground state energy using the variational method with a trial function \( \psi = e^{-\beta x^2/2} \).
Using the trial function \( \psi = e^{-\beta x^2/2} \) we find

\[
\langle H \rangle = \frac{\int_{-\infty}^{\infty} e^{-\beta x^2/2} \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2}{2\alpha} (1 - e^{-\alpha x^2}) \right] e^{-\beta x^2/2} dx}{\int_{-\infty}^{\infty} e^{-\beta x^2} dx}
\]

\[
= \hbar \omega \left[ \frac{1}{4} \left( \frac{\beta \hbar}{m\omega} \right) + \frac{m\omega}{2\hbar\alpha} \left( 1 - \frac{1}{\sqrt{1 + \alpha/\beta}} \right) \right]
\]

To find the value of \( \beta \) that minimizes the energy we set

\[
\frac{d \langle H \rangle}{d\beta} = 0
\]

We get

\[
\frac{d\langle H \rangle}{d\beta} = 0 = \frac{\hbar^2}{4m} - \frac{m\omega^2}{4\beta^2} \frac{1}{(1 + \alpha/\beta)^{3/2}}
\]

\[
\beta (1 + \alpha/\beta)^{3/4} = \frac{m\omega}{\hbar}
\]

Now \( \alpha \ll m\omega/\hbar \) gives the approximate zeroth-order solution

\[
\beta = \frac{m\omega}{\hbar}
\]

This gives

\[
\langle H \rangle = \hbar \omega \left[ \frac{1}{4} + \frac{m\omega}{2\hbar\alpha} \left( 1 - \frac{1}{\sqrt{1 + \alpha \hbar/m\omega}} \right) \right]
\]

which is the same as the result we got from first-order perturbation theory.

We can now iterate. We get

\[
\beta \left( 1 + \frac{\alpha}{(m\omega/\hbar)} \right)^{3/4} = \frac{m\omega}{\hbar} \Rightarrow \beta = \frac{m\omega}{\hbar} \left( 1 + \frac{\alpha \hbar}{m\omega} \right)^{-3/4}
\]

This gives a somewhat smaller value of \( \beta \) and a somewhat lower estimate (and thus better) for \( \langle H \rangle \).

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.

The unperturbed Hamiltonian of the system is two non-interacting hydrogen atoms so that

\[
\hat{H}_0 = -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2}
\]
with the ground-state wave function
\[ \psi_{100}(r) = \sqrt{\frac{2}{\pi a_0}} e^{-Zr/a_0}, \quad a_0 = \frac{\hbar^2}{me^2} \]

and
\[ E^{(0)} = -\frac{Z^2e^2}{2a_0} - \frac{Z^2e^2}{2a_0} = -\frac{Z^2e^2}{a_0} \]

Treating the e-e interaction
\[ V = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \]
as a perturbation, the first-order energy correction is
\[ E^{(1)} = \langle \varphi | V | \varphi \rangle = e^2 \int \frac{d^3r_1}{|\vec{r}_1 - \vec{r}_2|} |\psi_{100}(r_1)|^2 |\psi_{100}(r_2)|^2 \]
\[ = e^2 \left( \frac{Z^3}{\pi a_0^3} \right)^2 \int \frac{d^3r_1 d^3r_2}{|\vec{r}_1 - \vec{r}_2|^2} e^{-Z(r_1 + r_2)/a_0} = e^2 \left( \frac{Z^3}{\pi a_0^3} \right)^2 \frac{20\pi^2}{\left( \frac{2Z}{a_0} \right)^5} = \frac{5Ze^2}{8a_0} \]

so that the energy to first-order (for \( Z = 2 \) (helium)) is
\[ E = E^{(0)} + E^{(1)} = -\frac{Z^2e^2}{a_0} + \frac{5Ze^2}{8a_0} = -\frac{11e^2}{4a_0} \]

The ionization energy is the energy required to remove one electron of the helium atom to infinity. Therefore, for the ground state
\[ I = E_{hydrogen}^{Z=2} - E_{helium} = -\frac{Z^2e^2}{2a_0} + \frac{11e^2}{4a_0} = \frac{3e^2}{4a_0} \]

(b) Calculate the ionization energy by using the variational method with an effective charge \( \lambda \) in the hydrogenic wave function as the variational parameter.

For \( Z = 2 \) the Hamiltonian of helium including the e-e interaction is
\[ \hat{H} = -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \]

We will assume the trial function
\[ \varphi(r_1, r_2, \lambda) = \frac{\lambda^3}{\pi} e^{-\lambda(r_1 + r_2)} \]

Then the expectation value of the energy is given by
\[ E(\lambda) = \langle \varphi | H | \varphi \rangle \]
\[ = \int \int d^3r_1 d^3r_2 e^{-\lambda(r_1 + r_2)} \left( -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \right) \frac{\lambda^3}{\pi} e^{-\lambda(r_1 + r_2)} \]
Now

\[
\left( \frac{\lambda^3}{\pi} \right) \int d^3 \vec{r}_1 e^{-\lambda r_1} \left( -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{Z e^2}{r_1} \right) e^{-\lambda r_1} = \left( \frac{\lambda^3}{\pi} \right) \int d^3 \vec{r}_1 e^{-2\lambda r_1} \left( -\frac{\hbar^2}{2m} \frac{1}{r_1^2} \left( \frac{d}{dr_1} \frac{r_1^2}{dr_1} \right) - \frac{Z e^2}{r_1} \right) e^{-\lambda r_1} = \left( \frac{\lambda^3}{\pi} \right) \int d^3 \vec{r}_1 e^{-2\lambda r_1} \left( -\frac{\hbar^2}{2m} \left( \lambda^2 - \frac{2\lambda}{r_1} \right) - \frac{Z e^2}{r_1} \right) e^{-\lambda r_1} = \left( \frac{\lambda^3}{\pi} \right) \int d^3 \vec{r}_1 e^{-2\lambda r_1} \left( -\frac{\hbar^2}{2m} \left( \lambda^2 - \frac{2\lambda}{r_1} \right) - \frac{Z e^2 + \frac{\hbar^2 \lambda}{m}}{r_1} \right) e^{-\lambda r_1} = -\frac{\hbar^2 \lambda^2}{2m} - \left( \frac{\lambda^3}{\pi} \right) \int d^3 \vec{r}_1 e^{-2\lambda r_1} \left( \frac{Z e^2 + \frac{\hbar^2 \lambda}{m}}{r_1} \right) = -\frac{\hbar^2 \lambda^2}{2m} - 4\pi \left( \frac{\lambda^3}{\pi} \right) \left( Z e^2 + \frac{\hbar^2 \lambda}{m} \right) \int r_1 dr_1 e^{-2\lambda r_1} = -\frac{\hbar^2 \lambda^2}{2m} - 4\pi \left( \frac{\lambda^3}{\pi} \right) \left( Z e^2 + \frac{\hbar^2 \lambda}{m} \right) \frac{1}{4\lambda^2} \frac{\hbar^2 \lambda^2}{2m} - Z e^2 \lambda
\]

Therefore,

\[
\int \int d^3 \vec{r}_1 d^3 \vec{r}_2 \frac{\lambda^3}{\pi} e^{-\lambda (r_1 + r_2)} \left( -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) - \frac{Z e^2}{r_1} - \frac{Z e^2}{r_2} \right) \frac{\lambda^3}{\pi} e^{-\lambda (r_1 + r_2)} = 2 \left( \frac{\hbar^2 \lambda^2}{2m} - Z e^2 \lambda \right)
\]

and

\[
E(\lambda) = \frac{\hbar^2 \lambda^2}{m} - 2Z e^2 \lambda + \int \int d^3 \vec{r}_1 d^3 \vec{r}_2 \frac{\lambda^3}{\pi} e^{-\lambda (r_1 + r_2)} \left( \frac{e^2}{r_1^2 - r_2^2} \right) \frac{\lambda^3}{\pi} e^{-\lambda (r_1 + r_2)} = \frac{\hbar^2 \lambda^2}{m} - 2Z e^2 \lambda + \frac{\lambda^6 20e^2 \pi^2}{(2\lambda)^5} = \frac{\hbar^2 \lambda^2}{m} - 2Z e^2 \lambda + \frac{5}{8} \lambda e^2 \lambda = \frac{\hbar^2 \lambda^2}{m} - \left( 2Z e^2 - \frac{5}{8} e^2 \right) \lambda
\]

We now find the minimum with respect to $\lambda$.

\[
\frac{dE(\lambda)}{d\lambda} = 0 = \frac{d}{d\lambda} \left( \frac{\hbar^2 \lambda^2}{m} - \left( 2Z e^2 - \frac{5}{8} e^2 \right) \lambda \right)
\]

or

\[
\lambda = \frac{me^2}{2\hbar^2} \left( 2Z - \frac{5}{8} \right)
\]

Therefore, the ground-state energy (for $Z = 2$) is

\[
E = - \left( Z - \frac{5}{16} \right)^2 \frac{me^4}{\hbar^2} = - \left( \frac{27}{16} \right)^2 \frac{e^2}{a_0}
\]

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(c) Compare (a) and (b) with the experimental ionization energy

\[ E_{\text{ion}} = 1.807E_0 \quad , \quad E_0 = \frac{\alpha^2me^2}{2} \quad , \quad \alpha = \text{fine structure constant} \]

Finally, we have

\[ E_0^{PT} = -2.75\frac{e^2}{a_0} \quad , \quad E_0^{VAR} = -2.86\frac{e^2}{a_0} \quad , \quad E_0^{EXPT} = -2.90\frac{e^2}{a_0} \]

You will need

\[ \psi_{1s}(r) = \sqrt{\frac{\lambda^3}{\pi}} \exp(-\lambda r) \quad , \quad a_0 = \frac{\hbar^2}{me^2} \quad , \quad \int \int d^3r_1d^3r_2 e^{-\beta (r_1+r_2)} |\vec{r}_1 - \vec{r}_2| = \frac{20\pi^2}{\beta^5} \]

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

\[ V_{\text{pert}} = f(r)xy \]

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 \(\Delta E\), for one of the levels, what are the values of the shifts for all the others?

The four degenerate unperturbed wave functions are

\[ \langle \vec{r} | 2, 0, 0 \rangle = R_{20}(r)Y_{0,0}(\theta, \phi) \]
\[ \langle \vec{r} | 2, 1, 1 \rangle = R_{21}(r)Y_{1,1}(\theta, \phi) \]
\[ \langle \vec{r} | 2, 1, 0 \rangle = R_{21}(r)Y_{1,0}(\theta, \phi) \]
\[ \langle \vec{r} | 2, 1, -1 \rangle = R_{21}(r)Y_{1,-1}(\theta, \phi) \]

They all correspond to the same unperturbed energy

\[ E_2^{(0)} = -\frac{e^2}{8a_0} \to \text{4-fold degenerate level} \]

We need to calculate the \(4 \times 4\) degenerate submatrix for the perturbation

\[ V = f(r)xy = f(r)r^2 \sin^2 \theta \sin \phi \cos \phi \]
with matrix elements

\[ V_{\ell' \ell m'; \ell m} = \langle \ell' m' | \hat{V} | \ell m \rangle \]

\[ = \int R_{2 \ell'}(r) R_{2 \ell}(r) r^4 f(r) dr \int Y_{\ell' m'}^*(\theta, \phi) Y_{\ell m}(\theta, \phi) \sin^3 \theta \sin \phi \cos \phi d\theta d\phi \]

The necessary spherical harmonics are

\[ Y_{0,0} = \frac{1}{\sqrt{4\pi}}, \quad Y_{1,1} = \left( \frac{3}{8\pi} \right)^{1/2} \sin \theta e^{i\phi} \]
\[ Y_{1,0} = \left( \frac{3}{2\pi} \right)^{1/2} \cos \theta, \quad Y_{1,-1} = \left( \frac{3}{8\pi} \right)^{1/2} \sin \theta e^{-i\phi} \]

Now the \( \phi \) integrations take the form

\[ \int_0^{2\pi} \sin \phi \cos \phi d\phi = 0 \]

or

\[ \int_0^{2\pi} e^{i(m-m')\phi} \sin \phi \cos \phi d\phi \]

which is zero unless

\[ m = 1 = -m' \quad \text{or} \quad m = -1 = -m' \]

Therefore, the only nonzero matrix elements are

\[ V_{1,-1;1,1} = V_{1,1;1,-1}^* \]

\[ = \int R_{21}(r) R_{21}(r) r^4 f(r) dr \int Y_{1,-1}^*(\theta, \phi) Y_{1,1}(\theta, \phi) \sin^3 \theta \sin \phi \cos \phi d\theta d\phi \]

\[ = \frac{3}{8\pi} \int_0^{\infty} R_{21}^2(r) r^4 f(r) dr \int_0^{\pi} \sin^5 \theta d\theta \int_0^{2\pi} \sin \phi \cos \phi e^{-2i\phi} d\phi = iA \]

where

\[ A = \frac{1}{5} \int_0^{\infty} R_{21}^2(r) r^4 f(r) dr \]

Therefore the \( V \) matrix look like

\[
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & iA \\
0 & 0 & -iA & 0 \\
\end{pmatrix}
\rightarrow \text{eigenvalues} = 0, 0, \pm A
\]

Therefore the original 4-fold degenerate level splits into three new levels with the remaining degeneracy as indicated.
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

\[ \hat{H} = A\hat{\vec{L}}^2 + B\hat{L}_z + C\hat{L}_y \]

Assuming that \( A, B \gg C \), use perturbation theory to lowest nonvanishing order to get approximate energy eigenvalues.

We have

\[ \hat{H} = \hat{\vec{A}}\hat{L}^2 + B\hat{L}_z + C\hat{L}_y \]

We choose the unperturbed basis states \( |L, M\rangle \) where

\[ \hat{\vec{L}}^2 |L, M\rangle = \hbar^2 L(L + 1) |L, M\rangle \]
\[ \hat{L}_z |L, M\rangle = M\hbar |L, M\rangle \]

We also have

\[ \hat{L}_y = \frac{\hat{L}_+ - \hat{L}_-}{2i} \]

where

\[ \hat{L}_\pm |L, M\rangle = \hbar \sqrt{L(L + 1) - M(M \pm 1)} |L, M\rangle \]

For \( A, B \gg C \), we choose

\[ \hat{H}_0 = \hat{\vec{A}}\hat{L}^2 + B\hat{L}_z \]
\[ \hat{\hat{V}} = C\hat{L}_y = C\frac{\hat{L}_+ - \hat{L}_-}{2i} \]

The unperturbed energies are given by

\[ \hat{H}_0 |L, M\rangle = \hat{\vec{A}}\hat{L}^2 |L, M\rangle + B\hat{L}_z |L, M\rangle \]
\[ = (\hbar^2 L(L + 1) + BM\hbar) |L, M\rangle = E^{(0)}_{LM} |L, M\rangle \]

These levels are non-degenerate.

The general matrix element of \( \hat{\hat{V}} \) is given by

\[ \langle L'M'|\hat{\hat{V}}|LM\rangle = \frac{C}{2i} \left( \langle L'M'|\hat{L}_+|LM\rangle - \langle L'M'|\hat{L}_-|LM\rangle \right) \]
\[ = \frac{C\hbar}{2i} \left( \sqrt{L(L + 1) - M(M + 1)} \delta_{L,L'L'}\delta_{M',M+1} \right. \]
\[ \left. - \sqrt{L(L + 1) - M(M - 1)} \delta_{L,L'}\delta_{M',M-1} \right) \]
Since the diagonal matrix elements are zero, we have no first-order corrections, that is, \( E_{LM}^{(1)} = 0 \).

The second-order corrections (non-degenerate levels) are given by

\[
E_{LM}^{(2)} = \frac{C^2\hbar^2}{4} \sum_{M' \neq M} \left| \sqrt{L(L+1) - M(M+1)} \delta_{L',L} \delta_{M',M+1} - \sqrt{L(L+1) - M(M-1)} \delta_{L',L} \delta_{M',M-1} \right|^2 \frac{E_{LM}^{(0)} - E_{LM'}^{(0)}}{E_{LM}^{(0)} - E_{LM'}^{(0)}}
\]

\[
= \frac{C^2\hbar^2}{4} \left( \frac{L(L+1) - M(M+1)}{-B\hbar} + \frac{L(L+1) - M(M-1)}{B\hbar} \right)
\]

\[
= \frac{C^2\hbar}{4B} (M(M+1) - M(M-1)) = \frac{C^2\hbar}{2B} M
\]

Therefore to second order

\[
E_{LM} = A\hbar^2 L(L+1) + BM\hbar + \frac{C^2\hbar}{2B} M
\]

Alternatively, this Hamiltonian arises from a configuration shown below:

Therefore, if we rotate the system to the new \( z' \)-axis along \( \vec{B}_0 \), we get

\[
\hat{H} = A\hat{L}^2 + B_0 \hat{L}_{z'} , \quad B_0 = \sqrt{B^2 + C^2}
\]

We can solve this problem exactly. We get

\[
E = A\hbar^2 L(L+1) + (B^2 + C^2)^2 M'\hbar
\]

where

\[
|L, M'\rangle = D \left( \frac{\pi}{2}, 0, 0 \right) |L, M\rangle = \sum_{M=-L}^{L} D^{(L)}_{M,M'} \left( \frac{\pi}{2}, 0, 0 \right) |L, M\rangle
\]

For \( B \gg C \) we have

\[
E = A\hbar^2 L(L+1) + BM'\hbar + \frac{C^2\hbar}{2B} M' , \quad M' \approx M
\]

which is the same result as above.
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 $\vec{E}$ is applied in the plane. Find the change in the energy levels to first and second order in the field.

Take the plane of the rotator to be the $xy$–plane with the electric field in the $x$–direction such that the rotator (in direction of dipole moment $\vec{p}$) makes an angle $\theta$ with respect to the electric field.

In the absence of the electric field, we have

$$ \hat{H} = \frac{1}{2I} \hat{L}_z^2 = -\frac{\hbar^2}{2I} \frac{d^2}{d\theta^2} $$

so that the Schrodinger equation is

$$ -\frac{\hbar^2}{2I} \frac{d^2}{d\theta^2} \psi = E \psi $$

which has solutions

$$ \psi_m(\theta) = \frac{1}{\sqrt{2\pi}} e^{im\theta} , \quad m = 0, \pm 1, \pm 2, \ldots $$

corresponding to energy levels

$$ E_m^{(0)} = \frac{\hbar^2 m^2}{2I} $$

When the electric field acts on the system and is small enough to be treated as a perturbation, then we have

$$ V = -\vec{p} \cdot \vec{E} = -pe \cos \theta $$

The first-order energy correction is

$$ E_m^{(1)} = \langle m | V | m \rangle = -\frac{pe}{2\pi} \int_0^{2\pi} \cos \theta d\theta = 0 $$

The second-order correction is

$$ E_m^{(2)} = \sum_{m' \neq m} \frac{|\langle m' | V | m \rangle|^2}{E_m^{(0)} - E_{m'}^{(0)}} $$
Since
\[
\langle m' | V | m \rangle = -\frac{p_e}{2\pi} 2\pi \int_0^{2\pi} e^{i(m-m')\theta} \cos \theta d\theta = -\frac{p_e}{4\pi} \int_0^{2\pi} (e^{i(m-m'+1)\theta} + e^{i(m-m'-1)\theta}) d\theta
\]
we have for \( m \neq 0 \)
\[
E_m^{(2)} = \frac{p^2 e^2 \alpha}{4 \hbar^2} \left( \frac{1}{m^2 - (m-1)^2} + \frac{1}{m^2 - (m+1)^2} \right)
\]
If \( m = 0 \), only the first term \( \delta_{m',m+1} \) is valid and we get
\[
E_0^{(2)} = -\frac{p^2 e^2 \alpha}{2\hbar^2}
\]

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.

We can write
\[
\hat{H}_0 = \alpha (\hat{S}_x^2 + \hat{S}_y^2 - \hat{S}_z^2) /\hbar^2 = \alpha (\hat{S}^2 - 2\hat{S}_z^2) /\hbar^2
\]
so that the eigenvectors of \( \hat{H}_0 \) are \( |S, M\rangle \) where \( S \) can be 0 or 1. We then have
\[
\hat{H}_0 |S, M\rangle = \alpha (\hat{S}^2 - 2\hat{S}_z^2) /\hbar^2 |S, M\rangle = \alpha (S(S+1) - 2M^2) |S, M\rangle
\]
or
\[
\hat{H}_0 |0, 0\rangle = \hat{H}_0 |1, 1\rangle = \hat{H}_0 |1, -1\rangle = 0
\]
\[
\hat{H}_0 |1, 0\rangle = 2\alpha |1, 0\rangle
\]
Thus, there are two eigenvalues of \( \hat{H}_0 \), namely 0, which is triply degenerate, and \( 2\alpha \), which is non-degenerate or simple.

The corresponding eigenvectors are
\[
|1, 1\rangle = |1/2\rangle_1 |1/2\rangle_2
|1, 0\rangle = \frac{1}{\sqrt{2}} (|1/2\rangle_1 |-1/2\rangle_2 + |-1/2\rangle_1 |1/2\rangle_2)
|1, -1\rangle = |-1/2\rangle_1 |-1/2\rangle_2
|0, 0\rangle = \frac{1}{\sqrt{2}} (|1/2\rangle_1 |-1/2\rangle_2 - |-1/2\rangle_1 |1/2\rangle_2)
\]
(b) Consider the perturbation $\hat{H}_1 = \lambda (\hat{S}_{1x} - \hat{S}_{2x})$. Calculate the new energies in first-order perturbation theory.

Since

\[
\hat{S}_x |1/2\rangle = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2} |1/2\rangle
\]

and similarly,

\[
\hat{S}_x |-1/2\rangle = \frac{\hbar}{2} |-1/2\rangle
\]

it then follows that

\[
\hat{H}_1 |1,1\rangle = \lambda (\hat{S}_{1x} - \hat{S}_{2x}) |1,1\rangle = \lambda (\hat{S}_{1x} - \hat{S}_{2x}) |1/2\rangle_1 |1/2\rangle_2
\]

\[
= \frac{\lambda \hbar}{2} (|1/2\rangle_1 |1/2\rangle_2 - |1/2\rangle_2 |1/2\rangle_1) = -\frac{\lambda \hbar}{\sqrt{2}} |0,0\rangle
\]

and similarly,

\[
\hat{H}_1 |1,0\rangle = \lambda (\hat{S}_{1x} - \hat{S}_{2x}) |1,0\rangle
\]

\[
= \lambda (\hat{S}_{1x} - \hat{S}_{2x}) \frac{1}{\sqrt{2}} (|1/2\rangle_1 |-1/2\rangle_2 + |-1/2\rangle_1 |1/2\rangle_2) = 0
\]

and

\[
\hat{H}_1 |1,-1\rangle = \lambda (\hat{S}_{1x} - \hat{S}_{2x}) |1,-1\rangle
\]

\[
= \lambda (\hat{S}_{1x} - \hat{S}_{2x}) |-1/2\rangle_1 |-1/2\rangle_2 = \frac{\lambda \hbar}{\sqrt{2}} |0,0\rangle
\]

Therefore, $|1,0\rangle \hat{H}_1 |1,0\rangle = 0$, which means that the eigenvector, $|1,0\rangle$, of energy $2\alpha$, is not shifted by the perturbation, to first order. Among the matrix elements involving the degenerate eigenvectors, the only nonzero ones are

\[
\langle 0,0 | \hat{H}_1 |1,-1\rangle = \frac{\lambda \hbar}{\sqrt{2}} = -\langle 0,0 | \hat{H}_1 |1,1\rangle
\]

and their Hermitian conjugates. Accordingly, the perturbed energy levels are given by the characteristic equation

\[
\begin{vmatrix}
-E & -\frac{\lambda \hbar}{\sqrt{2}} & 0 \\
-\frac{\lambda \hbar}{\sqrt{2}} & -E & \frac{\lambda \hbar}{\sqrt{2}} \\
0 & \frac{\lambda \hbar}{\sqrt{2}} & -E
\end{vmatrix} = 0 = -E(E^2 - \lambda^2 \hbar^2) \rightarrow E = 0, \pm \lambda \hbar
\]

Therefore, the energy levels are shifted in this way:

\[
0(3 - fold) \Rightarrow 0, \pm \lambda \hbar \text{ (no remaining degeneracy)}
\]

\[
2\alpha \Rightarrow 2\alpha \text{ (unshifted)}
\]

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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 \( \hat{H}_0 \)

We have the unperturbed states and energies for

\[
\begin{align*}
\hat{H}_0 &= -A(\hat{S}_{1z} + \hat{S}_{2z}) \\
|++\rangle, \quad &-Ah \\
|+-\rangle, \quad &0 \\
|--\rangle, \quad &Ah \\
|-+\rangle, \quad &0
\end{align*}
\]

(b) Calculate the exact eigenvalues of \( \hat{H}_0 + \hat{H}_1 \)

We can rewrite the perturbation as

\[
\hat{H}_1 = B(\hat{S}_{1x}\hat{S}_{2x} - \hat{S}_{1y}\hat{S}_{2y}) = B\left(\frac{\hat{S}_{1+} + \hat{S}_{1-} + \hat{S}_{2+} + \hat{S}_{2-}}{2i} - \frac{\hat{S}_{1+} - \hat{S}_{1-} + \hat{S}_{2+} - \hat{S}_{2-}}{2i}\right)
\]

We then have

\[
\begin{align*}
\hat{H}_1 |++\rangle &= \frac{1}{2} B\left(\hat{S}_{1+} + \hat{S}_{1-} + \hat{S}_{2+} + \hat{S}_{2-}\right) |++\rangle = \frac{1}{2} B\hat{S}_+ |++\rangle = \frac{1}{2} B\hbar^2|--\rangle \\
\hat{H}_1 |--\rangle &= \frac{1}{2} B\hbar^2 |++\rangle \\
\hat{H}_1 |+-\rangle &= 0 \\
\hat{H}_1 |-+\rangle &= 0
\end{align*}
\]

The last two states are eigenvectors of the total Hamiltonian \( \hat{H} = \hat{H}_0 + \hat{H}_1 \) with eigenvalue 0. Of course, one can replace them by any orthonormal combination, for example, the symmetric and antisymmetric states

\[
\frac{1}{\sqrt{2}} (|+-\rangle \pm |--\rangle)
\]

To obtain the other eigenvectors, consider the eigenvalue equation

\[
(\hat{H}_0 + \hat{H}_1) (\cos \theta |++\rangle + \sin \theta |--\rangle) = \lambda (\cos \theta |++\rangle + \sin \theta |--\rangle)
\]

and

\[
-Ah (\cos \theta |++\rangle - \sin \theta |--\rangle) + \frac{1}{2} B\hbar^2 (\cos \theta |--\rangle + \sin \theta |++\rangle) = \lambda (\cos \theta |++\rangle + \sin \theta |--\rangle)
\]

We then have

\[
-Ah \cos \theta + \frac{1}{2} B\hbar^2 \sin \theta = \lambda \cos \theta \rightarrow (Ah + \lambda) \cos \theta = \frac{1}{2} B\hbar^2 \sin \theta \\
Ah \sin \theta + \frac{1}{2} B\hbar^2 \cos \theta = \lambda \sin \theta \rightarrow (-Ah + \lambda) \sin \theta = \frac{1}{2} B\hbar^2 \cos \theta
\]
or
\[
\left( \frac{\hat{A}h + \lambda}{\frac{1}{2} B h^2} \right) \Rightarrow \lambda^2 - A^2 h^2 = \frac{1}{4} B^2 h^4 \Rightarrow \lambda = \pm \frac{\hbar}{2} \sqrt{4 A^2 + B^2 h^2}
\]

Now
\[
\lambda_- = -\frac{\hbar}{2} \sqrt{4 A^2 + B^2 h^2}
\]
corresponds to the ground state and we find the eigenvector as follows.
We have
\[
\frac{(\hat{A}h + \lambda_-)}{B h^2/2} = \tan \theta = \frac{(\hat{A}h - \frac{\hbar}{2} \sqrt{4 A^2 + B^2 h^2})}{B h^2/2}
\]
and
\[
|\lambda_- \rangle = \cos \theta |--\rangle + \sin \theta |--\rangle = C (|--\rangle + \tan \theta |--\rangle)
\]

Similarly,
\[
\lambda_+ = \frac{\hbar}{2} \sqrt{4 A^2 + B^2 h^2}
\]
corresponds to the highest energy state and
\[
\frac{(\hat{A}h + \lambda_+)}{B h^2/2} = \tan \theta = \frac{(\hat{A}h + \frac{\hbar}{2} \sqrt{4 A^2 + B^2 h^2})}{B h^2/2}
\]
in this case.

(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 (b).

From above
\[
\langle ++ | \hat{H}_1 | ++ \rangle = \langle -- | \hat{H}_1 | -- \rangle = \langle + - | \hat{H}_1 | + - \rangle = \langle - + | \hat{H}_1 | - + \rangle = 0
\]
so that the first order correction to the energy is zero. For the ground state, \(|++, +\rangle\) with unperturbed energy \(-A\hbar\), the only contribution in second-order comes from the term
\[
\langle -- | \hat{H}_1 | ++ \rangle = \frac{1}{2} B h^2
\]
and so, to second-order in \( B \), the ground state energy is
\[
-A\hbar + \frac{|\langle -- | \hat{H}_1 | ++ \rangle|^2}{(-A\hbar) - (A\hbar)} = -A\hbar - \frac{B^2 h^3}{8A}
\]
The exact energy is
\[
\lambda_- = -\frac{\hbar}{2} \sqrt{4 A^2 + B^2 h^2}
\]
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which corresponds (for $A \gg B$) to
\[
\lambda_- = -\hbar \sqrt{1 + \frac{B^2 \hbar^2}{4A^2}} \approx -\hbar \left(1 + \frac{B^2 \hbar^2}{8A^2}\right) = -\hbar - \frac{B^2 \hbar^3}{8A}
\]
which agrees with the second-order result.

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?

The radial part of the Schrödinger equation for the particle in the potential well is
\[
R'' + \frac{2}{r} R' + \left(k^2 - \frac{\ell(\ell + 1)}{r^2}\right) R = 0, \quad E = \frac{\hbar^2 k^2}{2m}
\]
The boundary condition is $R(r - R) = 0$. Introducing a dimensionless variable $\rho = kr$, we get
\[
\frac{d^2 R}{d\rho^2} + \frac{2}{\rho} \frac{dR}{d\rho} + \left(1 - \frac{\ell(\ell + 1)}{\rho^2}\right) R = 0
\]
This is the spherical Bessel function equation with solutions $j_\ell(\rho)$ that are finite for $\rho \to 0$. $j_\ell(\rho)$ is related to the Bessel functions by
\[
j_\ell(\rho) = \left(\frac{\pi}{2\rho}\right)^{1/2} J_{\ell+1/2}(\rho)
\]
The radial wave function is then
\[
R_{k\ell}(r) = C_{k\ell} j_\ell(kr), \quad C_{k\ell} = \text{normalization factor}
\]
The boundary condition requires that
\[
j_\ell(kR) = 0
\]
which has solutions
\[
kR = \alpha_{n\ell}, \quad n = 1, 2, \ldots
\]
where the $\alpha_{n\ell}$ is the $n^{th}$ zero of the $\ell^{th}$ order spherical Bessel function. Then the bound states of the particle have energies given by
\[
E_{n\ell} = \frac{\hbar^2}{2mR^2} \alpha_{n\ell}^2, \quad n = 1, 2, \ldots
\]

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For the ground state, $\ell = 0$, and

$$j_0(\rho) = \frac{\sin \rho}{\rho}$$

Therefore, the boundary condition says that

$$\sin kR = 0 \rightarrow kR = \alpha_{10} = \pi \rightarrow E_{10} = \frac{\hbar^2 \pi^2}{2mR^2}$$

(b) Suppose that a weak uniform magnetic field of strength $B$ is switched on. Calculate the shift in the ground state energy.

We take the direction of the magnetic field as the $z$–direction. Then the vector potential can be written

$$A_x = -\frac{By}{2}, \quad A_y = \frac{Bx}{2}, \quad A_z = 0$$

and

$$\hat{H} = \frac{1}{2m} \left( \left( \hat{p}_x + \frac{eB}{2c} \hat{y} \right)^2 + \left( \hat{p}_y - \frac{eB}{2c} \hat{x} \right)^2 + \hat{p}_z^2 \right) + V(r)$$

$$= \frac{1}{2m} \left( \hat{p}^2 - \frac{eB}{c} \hat{L}_y - \hat{y} \hat{p}_x + \frac{e^2B^2}{4c^2} (\hat{x}^2 + \hat{y}^2) \right) + V(r)$$

$$= \frac{1}{2m} \left( \hat{p}^2 - \frac{eB}{c} \hat{L}_z + \frac{e^2B^2}{4c^2} (\hat{x}^2 + \hat{y}^2) \right) + V(r)$$

Since the magnetic field is weak, we can treat the term

$$-\frac{eB}{c} \hat{L}_z + \frac{e^2B^2}{4c^2} (\hat{x}^2 + \hat{y}^2)$$

as a perturbation.

When the system is in the ground state $L = 0, L_z = 0$ so that we only need to consider the term

$$\frac{e^2B^2}{4c^2} (\hat{x}^2 + \hat{y}^2) = \frac{e^2B^2}{4c^2} r^2 \sin^2 \theta$$

The ground state wave function is

$$\psi(r, \theta, \phi) = j_0(kr)Y_{00} = \frac{C \sin kr}{\sqrt{4\pi kr}}$$

Normalizing we have

$$1 = C^2 \frac{1}{k^2} \int_0^R \sin^2 krdr = C^2 \frac{1}{k^2} \int_0^R \left( \frac{1}{2} - \frac{1}{2} \cos kr \right) dr = C^2 \frac{1}{k^2} \left( \frac{R}{2} \right) \rightarrow C = \sqrt{\frac{2k^2}{R}}$$
Therefore,

\[ \psi(r, \theta, \phi) = \sqrt{\frac{1}{2\pi R}} \sin kr \]

and the first-order energy correction is

\[ E^{(1)} = \frac{e^2 B^2}{8mc^2} \frac{1}{2\pi R} \int_0^R r^2 \sin^2 kr \, dr \int_0^\pi 2\pi \sin^3 \theta d\theta = \left( \frac{1}{3} - \frac{1}{2\pi^2} \right) \frac{e^2 B^2 R^2}{12mc^2} \]

where we have used

\[ \sin kR = 0 \rightarrow kR = \pi \]

(c) Suppose that, instead a weak uniform electric field of strength \(E\) 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.

The corresponding potential energy (the perturbation) is

\[ V = -e\varepsilon z = -e\varepsilon r \cos \theta \]

The shift of the ground state energy is then

\[ E^{(2)}_\varepsilon = \sum_{m \neq 0 \text{= ground state}} \frac{|V_m|^2}{E^{(0)}_0 - E^{(0)}_m} \]

But, \(E^{(0)}_0 < E^{(0)}_m\) (\(m \neq 0\)) which says that each term in the sum is less than zero. This implies that the second-order correction causes an energy decrease.

(d) If, instead, a very strong magnetic field of strength \(B\) is turned on, approximately what would be the ground state energy?

If we have a very strong magnetic field, instead of a weak field, then

\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{e^2 B^2}{8mc^2} (\hat{x}^2 + \hat{y}^2) \]

and the \(B^2\) term can no longer be considered as a perturbation. The particle is now treated as a 2-dimensional harmonic oscillator with

\[ \frac{1}{2} m\omega^2 = \frac{e^2 B^2}{8mc^2} \rightarrow \omega = \frac{eB}{2mc} \]
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 $\vec{E} = E\hat{e}_x$.

The unperturbed world is given by the $n = 2$ 4-fold degenerate level of hydrogen with
\[ E_2^{(0)} = -\frac{e^2}{8a_0} \]
and states in the $|L.M\rangle$ basis $|0,0\rangle, |1,1\rangle, |1,0\rangle, |1,-1\rangle$. The perturbation is given by
\[ \hat{V} = V_{\text{electric}} + V_{\text{magnetic}} \]
\[ = -\vec{p} \cdot \vec{\varepsilon} - \frac{e}{mc} \vec{p} \cdot \vec{A} = -e\vec{r} \cdot \vec{\varepsilon} - \frac{e}{mc} \vec{p} \cdot \vec{A} \]
\[ = -e\vec{r} \cdot \varepsilon \hat{e}_z - \frac{e}{mc} \vec{p} \cdot \vec{A} = -e\varepsilon \hat{x} - \frac{e}{mc} \vec{p} \cdot \vec{A} \]

Now, $\vec{B} = B\hat{e}_z$, which says that $\vec{A} = Br\hat{\phi}$ so that
\[ -\frac{e}{mc} \vec{p} \cdot \vec{A} = -\frac{e}{mc} p_y \hat{B} = -\frac{eB}{mc} \frac{\hbar}{i} \frac{\partial}{\partial \phi} = \frac{h\omega_c}{i} \frac{\partial}{\partial \phi} = \omega_c \hat{L}_z \], $\omega_c = -\frac{eB}{mc}$
and thus
\[ V = -e\varepsilon \hat{x} + \omega_c \hat{L}_z \]

In the $|L.M\rangle$ basis, the term $\omega_c \hat{L}_z$ is diagonal, that is,
\[ \langle L'M' | V_{\text{magnetic}} | L M \rangle = Mh\omega_c \delta_{L'L} \delta_{M'M} \rightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & h\omega_c & 0 \\ 0 & 0 & -h\omega_c \end{pmatrix} \]

Note: the order of the states is $|0,0\rangle, |1,0\rangle, |1,1\rangle, |1,-1\rangle$.

Now we define
\[ \varsigma = -e\varepsilon \langle 0,0 | \hat{x} | 1,1 \rangle = -e\varepsilon \langle 0,0 | \hat{x} | 1,-1 \rangle \]
All other matrix elements are zero. We can see this as shown below.
\[ \langle 0,0 | \hat{x} | 1,0 \rangle \propto \frac{1}{2\pi} \int_0^{2\pi} (e^{i\phi} + e^{-i\phi}) d\phi = 0 \]

Therefore, the full $V$ matrix in the degenerate subspace is
\[ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \varsigma & \varsigma \\ 0 & h\omega_c & 0 \\ 0 & \varsigma & 0 & -h\omega_c \end{pmatrix} \]
The eigenvalues are

\[ E_2^{(0)} - \Delta \quad \text{non-degenerate} \]

\[ E_2^{(0)} + \Delta \quad \text{non-degenerate} \]

\[ E_2^{(0)} \quad \text{2-fold degenerate} \]
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.

The Stark effect involves the electric field potential energy

\[ V = eεr \cos θ \]

The \( n = 3 \) level of hydrogen has energy

\[ E^{(0)} = E_3 = -\frac{e^2}{18a_0} \]

There are 9 degenerate states (ignoring spin) corresponding to

\[ \ell = 2, \ m = \pm 2, \pm 1, 0 \rightarrow 5 \text{ states} \]
\[ \ell = 1, \ m = \pm 1, 0 \rightarrow 3 \text{ states} \]
\[ \ell = 0, \ m = 0 \rightarrow 1 \text{ state} \]

We denote the zero-order state vectors as \(|ℓ,m\rangle\)

\[ |1⟩ = |2, 2⟩, \quad |2⟩ = |2, -2⟩, \quad |3⟩ = |2, 1⟩ \]
\[ |4⟩ = |1, 1⟩, \quad |5⟩ = |2, -1⟩, \quad |6⟩ = |1, -1⟩ \]
\[ |7⟩ = |2, 0⟩, \quad |8⟩ = |1, 0⟩, \quad |9⟩ = |0, 0⟩ \]

The degenerate submatrix is \( 9 \times 9 = 81 \) elements. Because it is Hermitian, there are 45 independent elements to determine.

Now \( \cos θ \propto Y_{10} \) so that each matrix element contains the factor

\[ \langle ℓm | Y_{10} | ℓ'm'⟩ = 0 \quad \text{unless} \quad m = m' \text{ and} \quad ℓ' = ℓ + 1 \]

These relations are called selection rules. (More about selection rules in Chapter 11.) They say that the only nonzero matrix elements of \( V \) are

\[ \langle 3 | V | 4⟩ = \langle 4 | V | 3⟩ = a, \quad \langle 5 | V | 6⟩ = \langle 6 | V | 5⟩ = b \]
\[ \langle 7 | V | 8⟩ = \langle 8 | V | 7⟩ = c, \quad \langle 8 | V | 9⟩ = \langle 9 | V | 8⟩ = d \]

We will evaluate the matrix elements later.

The matrix is

\[
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & c & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & c & 0 & d & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & d & 0 \\
\end{pmatrix}
\]
We have two $2 \times 2$ and one $3 \times 3$ submatrices to diagonalize. The eigenvalues give the first-order energy corrections. We have

\[ E_{1}^{(1)}, E_{2}^{(1)} = 0 \quad 1x1 \text{ matrices} \]
\[ E_{3,4}^{(1)} = \pm a \quad 2x2 \text{ matrix} \]
\[ E_{5,6}^{(1)} = \pm b \quad 2x2 \text{ matrix} \]
\[ E_{7,8,9}^{(1)} = 0, \pm \sqrt{c^2 + d^2} \quad 3x3 \text{ matrix} \]

Calculation of matrix elements:

Radial/Angular functions:

\[ R_{32}(r) = \frac{2\sqrt{2}}{27\sqrt{3}} \left( \frac{1}{3a_0} \right)^{3/2} \left( \frac{r}{a_0} \right)^2 e^{-r/3a_0} \]
\[ R_{31}(r) = \frac{4\sqrt{2}}{9} \left( \frac{r}{a_0} \right)^{3/2} \left( 1 - \frac{r}{a_0} \right) e^{-r/3a_0} \]
\[ R_{30}(r) = 2 \left( \frac{1}{3a_0} \right)^{3/2} \left( 1 - \frac{2r}{3a_0} + \frac{a_0^2}{3a_0^2} \right) e^{-r/3a_0} \]

\[ Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} e^{\pm 2i\phi} \sin^2 \theta \quad , \quad Y_{2,\pm 1} = -\sqrt{\frac{15}{8\pi}} e^{\pm i\phi} \sin \theta \cos \theta \]
\[ Y_{2,0} = \sqrt{\frac{5}{16\pi}} (3\cos^2 \theta - 1) \quad , \quad Y_{1,\pm 1} = -\sqrt{\frac{3}{8\pi}} e^{\pm i\phi} \sin \theta \]
\[ Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos \theta \quad , \quad Y_{0,0} = \sqrt{\frac{1}{4\pi}} \]

Now

\[ a = \langle 4 | V | 3 \rangle = \langle 11 | V | 21 \rangle = e\varepsilon \int \int \int r^2 dr d\phi (\cos \theta) r \cos \theta R_{31} R_{32} Y_{11}^* Y_{21} \]

\[ = e\varepsilon \frac{2\sqrt{2}}{27\sqrt{3}} \left( \frac{1}{3a_0} \right)^{3/2} \frac{4\sqrt{2}}{9} \sqrt{3} \sqrt[6]{\frac{15}{8\pi}} \int_0^\infty \int_0^{2\pi} \int_0^{2\pi} e^{-2r/3a_0} dr d\phi e^{-i\phi} e^{+i\phi} d(\cos \theta) \sin^2 \theta \cos^2 \theta \]

\[ = e\varepsilon a_0 \frac{2}{3\pi} \left( \int_0^\infty x \left( 1 - \frac{x}{6} \right) e^{-2x/3} dx \right) \left( \int_0^{2\pi} d\phi \right) \left( \int_1^1 dy(1 - y^2) y^2 \right) \]

\[ = e\varepsilon a_0 \frac{2}{3\pi} (2\pi) \left( \int_0^\infty x^6 e^{-2x/3} dx - \frac{1}{6} \int_0^\infty x^7 e^{-2x/3} dx \right) \left( -\frac{4}{15} \right) \]

\[ = -e\varepsilon a_0 \frac{16}{5} \cdot \frac{3^8}{2} \left( \int_0^\infty x^6 e^{-2x/3} dx - \frac{1}{6} \int_0^\infty x^7 e^{-2x/3} dx \right) \]

\[ = -e\varepsilon a_0 \frac{16}{5} \cdot \frac{3^8}{2} \left( \frac{6!}{(\frac{3}{2})^7} - \frac{1}{6} \frac{7!}{(\frac{3}{2})^8} \right) = \frac{9}{2} e\varepsilon a_0 \]
Similarly,
\[ b = \frac{9}{2} \epsilon \alpha_0, \quad c = 3\sqrt{3} \epsilon \alpha_0, \quad d = 3\sqrt{6} \epsilon \alpha_0 \]

Therefore, the energy levels to first-order are
\[
E = -\frac{e^2}{18\alpha_0} \quad (3 \text{-fold degenerate})
\]
\[
E = -\frac{e^2}{18\alpha_0} + \frac{9}{2} \epsilon \alpha_0 \quad (2 \text{-fold degenerate})
\]
\[
E = -\frac{e^2}{18\alpha_0} - \frac{9}{2} \epsilon \alpha_0 \quad (2 \text{-fold degenerate})
\]
\[
E = -\frac{e^2}{18\alpha_0} + 9\epsilon \alpha_0 \quad \text{(non-degenerate)}
\]
\[
E = -\frac{e^2}{18\alpha_0} - 9\epsilon \alpha_0 \quad \text{(non-degenerate)}
\]

There are 5 new levels to first-order (one level remains 3-fold degenerate, two levels remain 2-fold degenerate and two levels are non-degenerate).

**Zero-order state vectors:**

\[
\begin{align*}
|1\rangle &= |1\rangle, \quad E = -\frac{e^2}{18\alpha_0} \\
|2\rangle &= |2\rangle, \quad E = -\frac{e^2}{18\alpha_0} \\
|3\rangle &= \frac{1}{\sqrt{2}} (|3\rangle + |4\rangle), \quad E = -\frac{e^2}{18\alpha_0} - \frac{9}{2} \epsilon \alpha_0 \\
|4\rangle &= \frac{1}{\sqrt{2}} (|3\rangle - |4\rangle), \quad E = -\frac{e^2}{18\alpha_0} + \frac{9}{2} \epsilon \alpha_0 \\
|5\rangle &= \frac{1}{\sqrt{2}} (|5\rangle + |6\rangle), \quad E = -\frac{e^2}{18\alpha_0} - \frac{9}{2} \epsilon \alpha_0 \\
|6\rangle &= \frac{1}{\sqrt{2}} (|5\rangle - |6\rangle), \quad E = -\frac{e^2}{18\alpha_0} + \frac{9}{2} \epsilon \alpha_0 \\
|7\rangle &= \sqrt{\frac{1}{6}} |7\rangle - \sqrt{\frac{1}{3}} |8\rangle + \sqrt{\frac{1}{3}} |9\rangle, \quad E = -\frac{e^2}{18\alpha_0} - 9\epsilon \alpha_0 \\
|8\rangle &= -\sqrt{\frac{2}{3}} |7\rangle + \sqrt{\frac{1}{3}} |9\rangle, \quad E = -\frac{e^2}{18\alpha_0} \\
|9\rangle &= \sqrt{\frac{1}{6}} |7\rangle + \sqrt{\frac{1}{2}} |8\rangle + \sqrt{\frac{1}{3}} |9\rangle, \quad E = -\frac{e^2}{18\alpha_0} + 9\epsilon \alpha_0
\end{align*}
\]

If we choose the values $e^2 = 1 = \alpha_0$ so that
\[
E = -\frac{1}{18} \\
E = -\frac{1}{18} + \frac{9}{2} \epsilon \\
E = -\frac{1}{18} - \frac{9}{2} \epsilon \\
E = -\frac{1}{18} + 9 \epsilon \\
E = -\frac{1}{18} - 9 \epsilon
\]

we get a plot that looks like:
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

$$\hat{H}_0 = \frac{\vec{p}^2}{2m} + V(r), \quad V(r) = -\frac{e^2}{r} \left( \frac{1}{r} \right)$$

$$\hat{H}_{so} = \left[ \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \right] \vec{S}_{op} \cdot \vec{L}_{op}$$

$$\hat{H}_m = \frac{\mu_B}{\hbar} (\vec{L}_{op} + 2\vec{S}_{op}) \cdot \vec{B}$$

We have two possible choices for basis functions, namely,

$$|n\ell sm\rangle \quad \text{or} \quad |n\ell sm\rangle$$

The former are easy to write down as direct-product states

$$|n\ell sm\rangle = R_{n\ell}(r)Y_{m}^{\ell} (\theta, \varphi) \ |s, m\rangle$$

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 \times 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.

We have

\[
\hat{H}_0 = \frac{\hat{p}_m^2}{2m} + V(r), \quad V(r) = -e^2 \left(\frac{1}{r}\right)
\]

\[
\hat{H}_{so} = \frac{1}{2m^2 e^2 r} \frac{dV(r)}{dr} \hat{S}_m \cdot \hat{L}_m
\]

\[
\hat{H}_m = \frac{\mu_B}{\hbar} (\hat{L}_m + 2\hat{S}_m) \cdot \vec{B}/\hbar
\]

Consider the \( n = 3 \) level of hydrogen which has energy

\[
E^{(0)} = E_3 = -\frac{e^2}{18a_0}
\]

There are 18 degenerate states corresponding to

\[
\begin{align*}
\ell = 2, & \quad m = \pm 2, \pm 1, 0 \rightarrow 5 \text{ states} \\
\ell = 1, & \quad m = \pm 1, 0 \rightarrow 3 \text{ states} \\
\ell = 0, & \quad m = 0 \rightarrow 1 \text{ state} \\
s = 1/2, & \quad m_s = \pm 1/2 \rightarrow 2 \text{ states for each } \ell \text{ state}
\end{align*}
\]

We denote the zero-order state vectors as \( |\ell, m, m_s\rangle \).

\[
\begin{align*}
|1\rangle &= |0, 0, +\rangle, & |2\rangle &= |0, 0, -\rangle, & |3\rangle &= |1, 1, +\rangle, & |4\rangle &= |1, 1, -\rangle \\
|5\rangle &= |1, 0, +\rangle, & |6\rangle &= |1, 0, -\rangle, & |7\rangle &= |1, -1, +\rangle, & |8\rangle &= |1, -1, -\rangle \\
|9\rangle &= |2, 2, +\rangle, & |10\rangle &= |2, 2, -\rangle, & |11\rangle &= |2, 1, +\rangle, & |12\rangle &= |2, 1, -\rangle \\
|13\rangle &= |2, 0, +\rangle, & |14\rangle &= |2, 0, -\rangle, & |15\rangle &= |2, -1, +\rangle, & |16\rangle &= |2, -1, -\rangle \\
|17\rangle &= |2, -2, +\rangle, & |18\rangle &= |2, -2, -\rangle
\end{align*}
\]

The degenerate matrix is 18 \times 18 = 324 elements. Because it is Hermitian, there are 171 independent elements to determine.

The magnetic term

\[
\hat{H}_m = \mu_B (\hat{L}_m + 2\hat{S}_m) \cdot \vec{B}/\hbar
\]

is diagonal in this basis as shown below:

\[
\langle \ell', m', m'_s | \hat{H}_m | \ell, m, m_s \rangle = \mu_B B \langle \ell', m', m'_s | (\hat{L}_z + 2\hat{S}_z) | \ell, m, m_s \rangle
\]

\[
= \mu_B B (m + 2m_s) \delta_{\ell\ell'} \delta_{m'm} \delta_{m'_sm_s}
\]
The spin-orbit term

\[ \hat{H}_{so} = \left[ \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \right] \vec{S}_o \cdot \vec{L}_{op} \]

can be rewritten as

\[ \hat{H}_{so} = \left[ \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \right] \vec{S}_{op} \cdot \hat{L}_{op} = \left[ \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \right] \left( \hat{L}_z \hat{S}_z + \frac{1}{2} \left( \hat{L}_+ \hat{S}_- + \hat{L}_- \hat{S}_+ \right) \right) \]

This means that the matrix element

\[ \langle \ell', m', m'_s | \hat{H}_{so} | \ell, m, m_s \rangle \]

\[ = \langle \ell', m', m'_s | \left[ \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \right] \left( \hat{L}_z \hat{S}_z + \frac{1}{2} \left( \hat{L}_+ \hat{S}_- + \hat{L}_- \hat{S}_+ \right) \right) | \ell, m, m_s \rangle \]

equals zero unless one of the following conditions holds:

\( (m' = m & m'_s = m_s) \)

\( or \)

\( (m' + 1 = m & m'_s - 1 = m_s) \)

\( or \)

\( (m' + 1 = m & m'_s + 1 = m_s) \)

Therefore, we have to calculate all of the diagonal elements, but only the off-diagonal elements below:

\[ \langle 4 | \hat{H}_{so} | 5 \rangle , \langle 6 | \hat{H}_{so} | 7 \rangle , \langle 10 | \hat{H}_{so} | 11 \rangle , \langle 12 | \hat{H}_{so} | 13 \rangle , \langle 14 | \hat{H}_{so} | 15 \rangle , \langle 16 | \hat{H}_{so} | 17 \rangle \]
We also note that any diagonal element is zero if $m = 0$ and the matrix element is zero if $\ell = 0$.

Finally, we note that
\[
\left\langle \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \right\rangle_{nt} = \frac{e^2}{2m^2c^2} \left\langle n\ell \right| \frac{1}{r^3} \left| n\ell \right\rangle = \frac{e^2}{2m^2c^2} \left[ \frac{Z^3}{a_0^3} n! 3 \ell (\ell + 1/2)(\ell + 1) \right]
\]
where
\[
A = \frac{Z^3 e^2}{2m^2c^2 a_0^3} = \frac{e^2}{54m^2c^2 a_0^3}
\]

Therefore, we have
\[
\left\langle \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \right\rangle_{32} = \frac{A}{15}, \quad \left\langle \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \right\rangle_{31} = \frac{A}{3}
\]

So let us do it.....

\begin{align*}
\langle 1 | \hat{H}_{so} | 1 \rangle &= \langle 2 | \hat{H}_{so} | 2 \rangle = \langle 5 | \hat{H}_{so} | 5 \rangle = 0 \\
\langle 6 | \hat{H}_{so} | 6 \rangle &= \langle 13 | \hat{H}_{so} | 13 \rangle = \langle 14 | \hat{H}_{so} | 14 \rangle = 0 \\
\langle 3 | \hat{H}_{so} | 3 \rangle &= \frac{4}{3} \langle 1, 1, + | \hat{L}_z \hat{S}_z | 1, 1, + \rangle = \frac{4}{3} \left( \frac{\hbar^2}{2} \right) = \frac{4\hbar^2}{3} \\
\langle 4 | \hat{H}_{so} | 4 \rangle &= \frac{4}{3} \langle 1, 1, - | \hat{L}_z \hat{S}_z | 1, 1, - \rangle = \frac{4}{3} \left( - \frac{\hbar^2}{2} \right) = -\frac{4\hbar^2}{3} \\
\langle 4 | \hat{H}_{so} | 5 \rangle &= \frac{4}{6} \langle 1, 1, - | \hat{L}_+ \hat{S}_- | 1, 0, + \rangle = \frac{4}{6} \left( \sqrt{2}\hbar^2 \right) = \frac{\sqrt{2}\hbar^2}{6} \\
\langle 6 | \hat{H}_{so} | 7 \rangle &= \frac{4}{6} \langle 1, 0, - | \hat{L}_+ \hat{S}_- | 1, -1, + \rangle = \frac{4}{6} \left( \sqrt{2}\hbar^2 \right) = \frac{\sqrt{2}\hbar^2}{6} \\
\langle 7 | \hat{H}_{so} | 7 \rangle &= \frac{4}{6} \langle 1, -1, + | \hat{L}_z \hat{S}_z | 1, -1, + \rangle = \frac{4}{6} \left( \frac{\hbar^2}{2} \right) = -\frac{2\hbar^2}{3} \\
\langle 8 | \hat{H}_{so} | 8 \rangle &= \frac{4}{6} \langle 1, -1, - | \hat{L}_z \hat{S}_z | 1, -1, - \rangle = \frac{4}{6} \left( \frac{\hbar^2}{2} \right) = \frac{\hbar^2}{3} \\
\langle 9 | \hat{H}_{so} | 9 \rangle &= \frac{4}{15} \langle 2, 2, - | \hat{L}_z \hat{S}_z | 2, 2, + \rangle = \frac{4}{15} \left( \hbar^2 \right) = \frac{4\hbar^2}{15} \\
\langle 10 | \hat{H}_{so} | 10 \rangle &= \frac{4}{15} \langle 2, 2, - | \hat{L}_z \hat{S}_z | 2, 2, - \rangle = \frac{4}{15} \left( -\hbar^2 \right) = -\frac{4\hbar^2}{15} \\
\langle 10 | \hat{H}_{so} | 11 \rangle &= \frac{4}{15} \langle 2, 2, - | \hat{L}_+ \hat{S}_- | 2, 1, + \rangle = \frac{4}{15} \left( \frac{2\hbar^2}{3} \right) = \frac{2\hbar^2}{5} \\
\langle 11 | \hat{H}_{so} | 11 \rangle &= \frac{4}{15} \langle 2, 1, + | \hat{L}_z \hat{S}_z | 2, 1, + \rangle = \frac{4}{15} \left( \hbar^2 \right) = \frac{4\hbar^2}{30} \\
\langle 12 | \hat{H}_{so} | 12 \rangle &= \frac{4}{15} \langle 2, 1, - | \hat{L}_z \hat{S}_z | 2, 1, - \rangle = \frac{4}{15} \left( -\hbar^2 \right) = -\frac{4\hbar^2}{15} \\
\langle 13 | \hat{H}_{so} | 13 \rangle &= \frac{4}{30} \langle 2, 1, - | \hat{L}_+ \hat{S}_- | 2, 0, + \rangle = \frac{4}{30} \left( \frac{\sqrt{6}\hbar^2}{30} \right) = \frac{\sqrt{6}\hbar^2}{30} \\
\langle 14 | \hat{H}_{so} | 15 \rangle &= \frac{4}{30} \langle 2, 0, - | \hat{L}_+ \hat{S}_- | 2, 0, + \rangle = \frac{4}{30} \left( \sqrt{2}\hbar^2 \right) = \frac{2\hbar^2}{15} \\
\langle 15 | \hat{H}_{so} | 15 \rangle &= \frac{4}{15} \langle 2, 1, - | \hat{L}_z \hat{S}_z | 2, 1, - \rangle = \frac{4}{15} \left( -\frac{\hbar^2}{2} \right) = -\frac{2\hbar^2}{15} \\
\langle 16 | \hat{H}_{so} | 16 \rangle &= \frac{4}{15} \langle 2, 2, - | \hat{L}_z \hat{S}_z | 2, 2, - \rangle = \frac{4}{15} \left( \frac{\hbar^2}{2} \right) = \frac{2\hbar^2}{15} \\
\langle 16 | \hat{H}_{so} | 17 \rangle &= \frac{4}{30} \langle 2, 2, - | \hat{L}_+ \hat{S}_- | 2, 2, + \rangle = \frac{4}{30} \left( \frac{2\hbar^2}{3} \right) = \frac{\hbar^2}{15} \\
\langle 17 | \hat{H}_{so} | 17 \rangle &= \frac{4}{15} \langle 2, -2, + | \hat{L}_z \hat{S}_z | 2, -2, + \rangle = \frac{4}{15} \left( \frac{\hbar^2}{2} \right) = \frac{2\hbar^2}{15} \\
\langle 18 | \hat{H}_{so} | 18 \rangle &= \frac{4}{15} \langle 2, -2, - | \hat{L}_z \hat{S}_z | 2, -2, - \rangle = \frac{4}{15} \left( -\hbar^2 \right) = -\frac{4\hbar^2}{15}
\end{align*}
Therefore, the corresponding matrix is as below:

\[
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -5 & 5\sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 5\sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -5 & 5\sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 5\sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

\( \frac{Ah^2}{30} \)

\[
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

(b) Diagonalize the blocks and determine the eigenvalues as functions of \( B \).

We can read off the energies that are diagonal

\[
|1\rangle \to E^{(1)} = \mu_B B \\
|2\rangle \to E^{(1)} = -\mu_B B \\
|3\rangle \to E^{(1)} = \frac{Ah^2}{6} + 2\mu_B B \\
|8\rangle \to E^{(1)} = \frac{Ah^2}{6} - 2\mu_B B \\
|9\rangle \to E^{(1)} = \frac{Ah^2}{15} + 3\mu_B B \\
|18\rangle \to E^{(1)} = \frac{Ah^2}{15} - 3\mu_B B
\]

We then need to diagonalize these remaining six \( 2 \times 2 \) submatrices.

\[
4 - 5 \begin{pmatrix}
-5\frac{Ah^2}{30} & 5\sqrt{2}\frac{Ah^2}{30} \\
5\sqrt{2}\frac{Ah^2}{30} & \mu_B B
\end{pmatrix}
\]

\[
6 - 7 \begin{pmatrix}
-\mu_B B & 5\sqrt{2}\frac{Ah^2}{30} \\
5\sqrt{2}\frac{Ah^2}{30} & -5\frac{Ah^2}{30}
\end{pmatrix}
\]

\[
10 - 11 \begin{pmatrix}
-2\frac{Ah^2}{30} + \mu_B B & 2\frac{Ah^2}{30} \\
2\frac{Ah^2}{30} & -2\frac{Ah^2}{30} + 2\mu_B B
\end{pmatrix}
\]

\[
12 - 13 \begin{pmatrix}
-\frac{Ah^2}{30} & \sqrt{6}\frac{Ah^2}{30} \\
\sqrt{6}\frac{Ah^2}{30} & \mu_B B
\end{pmatrix}
\]
\[
14 - 15 \left( \frac{-\mu_B B}{\sqrt[6]{A h^2_{30}}} \sqrt[6]{A h^2_{30}} - \frac{6 A h^2_{30}}{10} \right)
\]
\[
16 - 17 \left( \frac{A h^2_{30} - 2 \mu_B B}{2 A h^2_{30} - \mu_B B} \right)
\]

We get characteristic equations:

\[
4 - 5 \left( \frac{-5 A h^2_{30}}{2 A h^2_{30} - \mu_B B} \right) \rightarrow (E - \mu_B B)(E + \frac{A h^2}{6}) - \frac{1}{18} (A h^2)^2 = 0
\]
\[
6 - 7 \left( \frac{-\mu_B B}{2 A h^2_{30} - \mu_B B} \right) \rightarrow (E + \mu_B B)(E + \frac{A h^2}{6}) - \frac{1}{18} (A h^2)^2 = 0
\]
\[
10 - 11 \left( \frac{-2 A h^2_{30} + \mu_B B}{2 A h^2_{30}} \right) \rightarrow (E - \mu_B B + \frac{A h^2}{15})(E - \frac{A h^2}{30} - 2 \mu_B B) = \left( \frac{A h^2}{15} \right)^2 = 0
\]
\[
12 - 13 \left( \frac{-\mu_B B}{2 A h^2_{30}} \right) \rightarrow (E - \mu_B B)(E + \frac{A h^2}{30}) - \frac{1}{150} (A h^2)^2 = 0
\]
\[
14 - 15 \left( \frac{-A h^2_{30}}{2 A h^2_{30} - \mu_B B} \right) \rightarrow (E + \mu_B B)(E + \frac{A h^2}{30}) - \frac{1}{150} (A h^2)^2 = 0
\]
\[
16 - 17 \left( \frac{A h^2_{30} - 2 \mu_B B}{2 A h^2_{30} - \mu_B B} \right) \rightarrow (E + \mu_B B + \frac{A h^2}{15})(E + 2 \mu_B B - \frac{A h^2}{30}) = \left( \frac{A h^2}{15} \right)^2 = 0
\]

Continuing .......

\[
E = \frac{1}{2} \left( \mu_B B - \frac{A h^2}{6} \right) \pm \frac{1}{2} \sqrt{\left( \frac{\mu_B B}{A h^2_{30}} \right) + \frac{2}{9} (A h^2)^2 + \mu_B B \frac{2 A h^2_{30}}{3}}
\]
\[
e = \frac{1}{2} \left( \mu_B B - \frac{A h^2}{6} \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} (A h^2)^2 + \frac{1}{3} \mu_B B A h^2 + (\mu_B B)^2}
\]

\[
E = -\frac{1}{2} \left( \frac{A h^2}{6} + \mu_B B \right) \pm \frac{1}{2} \sqrt{\left( \frac{A h^2}{6} + \mu_B B \right)^2 + \frac{2}{9} (A h^2)^2 - \mu_B B \frac{2 A h^2_{30}}{3}}
\]
\[
e = -\frac{1}{2} \left( \frac{A h^2}{6} + \mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} (A h^2)^2 - \frac{1}{3} \mu_B B A h^2 + (\mu_B B)^2}
\]

\[
E = \frac{1}{2} \left( \frac{A h^2_{30} - 3 \mu_B B}{30} \right) \pm \sqrt{\left( \frac{A h^2_{30} - 3 \mu_B B}{30} \right)^2 + 4 \left( \frac{A h^2}{15} \right)^2 + 4 \left( \frac{A h^2_{30}}{30} + 2 \mu_B B \right) \left( \frac{A h^2}{15} - \mu_B B \right)}
\]
\[
e = \frac{1}{2} \left( \frac{A h^2_{30} - 3 \mu_B B}{30} \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} (A h^2)^2 + \frac{1}{5} \mu_B B A h^2 + (\mu_B B)^2}
\]

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12-13

\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} + \mu_B B \right) \pm \frac{1}{2} \sqrt{\left( \frac{Ah^2}{30} + \mu_B B \right)^2 + 4 \frac{1}{150} \left( \frac{Ah^2}{15} \right)^2 + 4 \mu_B B A \frac{Ah^2}{30} + (\mu_B B)^2} \]

14-15

\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} + \mu_B B \right) \pm \frac{1}{2} \sqrt{\left( \frac{Ah^2}{30} + \mu_B B \right)^2 + 4 \frac{1}{150} \left( \frac{Ah^2}{15} \right)^2 - 4 \mu_B B A \frac{Ah^2}{30} + (\mu_B B)^2} \]

16-17

\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} + 3\mu_B B \right) \pm \frac{1}{2} \sqrt{\left( \frac{Ah^2}{30} + 3\mu_B B \right)^2 + 4 \left( \frac{Ah^2}{15} \right)^2 + 4 \left( \frac{Ah^2}{15} + \mu_B B \right) \left( \frac{Ah^2}{30} - 2\mu_B B \right)} \]

(c) Look at the \( B \to 0 \) limit. Identify the spin-orbit levels. Characterize them by \((\ell s_j)\).

The \( B \to 0 \) limit:

4-5

\[ E = \frac{1}{2} \left( \mu_B B - \frac{Ah^2}{6} \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} \left( Ah^2 \right)^2 + \frac{1}{3} \mu_B B Ah^2 + (\mu_B B)^2} \]

\[ \to \frac{1}{6} Ah^2 + \frac{2}{3} \mu_B B , \ -\frac{1}{4} Ah^2 + \frac{1}{4} \mu_B B \]

6-7

\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} - \frac{Ah^2}{6} \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} \left( Ah^2 \right)^2 - \frac{1}{3} \mu_B B Ah^2 + (\mu_B B)^2} \]

\[ \to \frac{1}{6} Ah^2 - \frac{2}{3} \mu_B B , \ -\frac{1}{3} Ah^2 - \frac{1}{3} \mu_B B \]

10-11

\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} - 3\mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} \left( Ah^2 \right)^2 + \frac{1}{3} \mu_B B Ah^2 + (\mu_B B)^2} \]

\[ \to \frac{1}{15} Ah^2 + \frac{2}{5} \mu_B B , \ -\frac{1}{15} Ah^2 + \frac{2}{5} \mu_B B \]

12-13

\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} - \mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} \left( Ah^2 \right)^2 + \frac{1}{15} \mu_B B Ah^2 + (\mu_B B)^2} \]

\[ \to \frac{1}{15} Ah^2 + \frac{2}{5} \mu_B B , \ -\frac{1}{15} Ah^2 + \frac{2}{5} \mu_B B \]

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14-15
\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} + \mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} (Ah^2)^2 - \frac{1}{4} \mu_B B Ah^2 + (\mu_B B)^2} \]
\[ \rightarrow \frac{1}{15} Ah^2 - \frac{3}{5} \mu_B B, \quad -\frac{1}{15} Ah^2 - \frac{3}{5} \mu_B B \]

16-17
\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} + 3\mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} (Ah^2)^2 - \frac{1}{4} \mu_B B Ah^2 + (\mu_B B)^2} \]
\[ \rightarrow \frac{1}{15} Ah^2 - \frac{9}{5} \mu_B B, \quad -\frac{1}{15} Ah^2 - \frac{6}{5} \mu_B B \]

Spin-Orbit Levels

These levels go like
\[ \frac{Ah^2 (j(j + 1) - \ell(\ell + 1) - s(s + 1))}{2 \ell(\ell + 1/2)(\ell + 1)} \]

so that
\[ 0 \rightarrow |1\rangle, |2\rangle \rightarrow \ell = 0, \quad s = 1/2, \quad j = 1/2 \]
\[ +\frac{Ah^2}{6} \rightarrow |3\rangle, |8\rangle, |4\rangle, |6\rangle \rightarrow \ell = 1, \quad s = 1/2, \quad j = 3/2 \]
\[ +\frac{Ah^2}{10} \rightarrow |9\rangle, |18\rangle, |16\rangle, |14\rangle, |16\rangle \rightarrow \ell = 2, \quad s = 1/2, \quad j = 5/2 \]
\[ -\frac{Ah^2}{3} \rightarrow |5\rangle, |7\rangle \rightarrow \ell = 1, \quad s = 1/2, \quad j = 1/2 \]
\[ -\frac{Ah^2}{10} \rightarrow |11\rangle, |13\rangle, |15\rangle, |17\rangle \rightarrow \ell = 2, \quad s = 1/2, \quad j = 3/2 \]
in agreement with the spin-orbit formula.

(d) Look at the large \( B \) limit. Identify the Paschen-Bach levels.

The \( B \rightarrow \infty \) limit:
\[ |1\rangle \rightarrow +\mu_B B \]
\[ |2\rangle \rightarrow -\mu_B B \]
\[ |3\rangle \rightarrow +2\mu_B B \]
\[ |8\rangle \rightarrow -2\mu_B B \]
\[ |9\rangle \rightarrow +3\mu_B B \]
\[ |18\rangle \rightarrow -3\mu_B B \]

4-5
\[ E = \frac{1}{2} \left( \mu_B B - \frac{Ah^2}{6} \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} (Ah^2)^2 + \frac{1}{3} \mu_B B Ah^2 + (\mu_B B)^2} \rightarrow \mu_B B, \quad 0 \]

6-7
\[ E = -\frac{1}{2} \left( \frac{Ah^2}{6} + \mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} (Ah^2)^2 - \frac{1}{3} \mu_B B Ah^2 + (\mu_B B)^2} \rightarrow 0, \quad -\mu_B B \]

10-11
\[ E = \frac{1}{2} \left( \frac{Ah^2}{30} - 3\mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} (Ah^2)^2 + \frac{1}{5} \mu_B B Ah^2 + (\mu_B B)^2} \rightarrow 2\mu_B B, \quad \mu_B B \]
12-13

\[ E = \frac{1}{2} \left( \frac{Ah^2}{30} - \mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} (Ah^2)^2 + \frac{1}{15} \mu_B B Ah^2 + (\mu_B B)^2} \rightarrow \mu_B B , \ 0 \]

14-15

\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} + \mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} (Ah^2)^2 - \frac{1}{15} \mu_B B Ah^2 + (\mu_B B)^2} \rightarrow 0 , \ -\mu_B B \]

16-17

\[ E = -\frac{1}{2} \left( \frac{Ah^2}{30} + 3\mu_B B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} (Ah^2)^2 - \frac{1}{5} \mu_B B Ah^2 + (\mu_B B)^2} \rightarrow -\mu_B B , \ -2\mu_B B \]

The Paschen-Back levels are

\[
\begin{align*}
3\mu_B B & \rightarrow |9\rangle \\
2\mu_B B & \rightarrow |3\rangle, |10\rangle \\
\mu_B B & \rightarrow |1\rangle, |1\rangle, |1\rangle, |1\rangle \\
0 & \rightarrow |5\rangle, |6\rangle, |13\rangle, |14\rangle \\
-\mu_B B & \rightarrow |2\rangle, |7\rangle, |15\rangle, |16\rangle \\
-2\mu_B B & \rightarrow |8\rangle, |17\rangle \\
-3\mu_B B & \rightarrow |18\rangle
\end{align*}
\]

Thus we have 7 equally spaced levels.

(e) For small \( B \) show the Zeeman splittings and identify the Lande \( g \)-factors.

Limit \( B \gg A \): Zeeman effect

\[
\begin{align*}
|1\rangle, |2\rangle & \rightarrow \ell = 0 , \ s = 1/2 , \ j = 1/2 \\
|3\rangle, |8\rangle, |4\rangle, |6\rangle & \rightarrow \ell = 1 , \ s = 1/2 , \ j = 3/2 \\
|9\rangle, |18\rangle, |10\rangle, |12\rangle, |14\rangle, |16\rangle & \rightarrow \ell = 2 , \ s = 1/2 , \ j = 5/2 \\
|5\rangle, |7\rangle & \rightarrow \ell = 1 , \ s = 1/2 , \ j = 1/2 \\
|11\rangle, |13\rangle, |15\rangle, |17\rangle & \rightarrow \ell = 2 , \ s = 1/2 , \ j = 3/2
\end{align*}
\]

The Lande-g factor is

\[
g = 1 + \frac{j(j + 1) + s(s + 1) - \ell(\ell + 1)}{2j(j + 1)}
\]

The levels go like: \( E_{so} + gm_j \mu_B B \)

\[
\begin{align*}
|1\rangle, |2\rangle & \rightarrow \ell = 0 , \ s = 1/2 , \ j = 1/2 \rightarrow g = 2 \\
|3\rangle, |8\rangle, |4\rangle, |6\rangle & \rightarrow \ell = 1 , \ s = 1/2 , \ j = 3/2 \rightarrow g = 4/3 \\
|9\rangle, |18\rangle, |10\rangle, |12\rangle, |14\rangle, |16\rangle & \rightarrow \ell = 2 , \ s = 1/2 , \ j = 5/2 \rightarrow g = 6/5 \\
|5\rangle, |7\rangle & \rightarrow \ell = 1 , \ s = 1/2 , \ j = 1/2 \rightarrow g = 2/3 \\
|11\rangle, |13\rangle, |15\rangle, |17\rangle & \rightarrow \ell = 2 , \ s = 1/2 , \ j = 3/2 \rightarrow g = 4/5
\end{align*}
\]
\[ |1\rangle \rightarrow \mu_B B \rightarrow gm_j = (2) (1/2) \]
\[ |2\rangle \rightarrow -\mu_B B \rightarrow gm_j = (2) (-1/2) \]
\[ |3\rangle \rightarrow \frac{\Delta h^2}{\mu_B} + 2\mu_B B \rightarrow gm_j = (4/3) (3/2) \]
\[ |8\rangle \rightarrow \frac{\Delta h^2}{\mu_B} - 2\mu_B Bb \rightarrow gm_j = (4/3) (-3/2) \]
\[ |9\rangle \rightarrow \frac{\Delta h^2}{\mu_B} + 3\mu_B B \rightarrow gm_j = (6/5) (5/2) \]
\[ |18\rangle \rightarrow \frac{\Delta h^2}{\mu_B} - 3\mu_B B \rightarrow gm_j = (6/5) (-5/2) \]

4-5
\[ \frac{1}{6} Ah^2 + \frac{2}{3} \mu_B B , \quad \frac{1}{3} Ah^2 + \frac{1}{3} \mu_B B \rightarrow gm_j = (4/3) (1/2) , \quad (2/3) (1/2) \]

6-7
\[ \frac{1}{6} Ah^2 - \frac{2}{3} \mu_B B , \quad \frac{1}{3} Ah^2 - \frac{1}{3} \mu_B B \rightarrow gm_j = (4/3) (-1/2) , \quad (2/3) (-1/2) \]

10-11
\[ \frac{1}{15} Ah^2 + \frac{9}{5} \mu_B B , \quad \frac{1}{10} Ah^2 + \frac{6}{5} \mu_B B \rightarrow gm_j = (6/5) (3/2) , \quad (4/5) (3/2) \]

12-13
\[ \frac{1}{15} Ah^2 + \frac{3}{5} \mu_B B , \quad \frac{1}{10} Ah^2 + \frac{2}{5} \mu_B B \rightarrow gm_j = (6/5) (1/2) , \quad (4/5) (1/2) \]

14-15
\[ \frac{1}{15} Ah^2 - \frac{3}{5} \mu_B B , \quad \frac{1}{10} Ah^2 - \frac{2}{5} \mu_B B \rightarrow gm_j = (6/5) (-1/2) , \quad (4/5) (-1/2) \]

16-17
\[ \frac{1}{15} Ah^2 - \frac{9}{5} \mu_B B , \quad \frac{1}{10} Ah^2 - \frac{6}{5} \mu_B B \rightarrow gm_j = (6/5) (-3/2) , \quad (4/5) (-3/2) \]

so that the results are in agreement with the Lande-g factor formula.

(f) Plot the eigenvalues versus $B$. We choose $\mu_B = 1 = Ah^2$ so that the energy levels become

\[ |1\rangle \rightarrow E = B \]
\[ |2\rangle \rightarrow E = -B \]
\[ |3\rangle \rightarrow E = \frac{1}{6} + 2B \]
\[ |8\rangle \rightarrow E = \frac{1}{6} - 2B \]
\[ |9\rangle \rightarrow E = \frac{1}{16} + 3B \]
\[ |18\rangle \rightarrow E = \frac{1}{16} - 3B \]

4-5
\[ E = \frac{1}{2} \left( B - \frac{1}{6} \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} + \frac{1}{3} B + B^2} \]

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\[ E = -\frac{1}{2} \left( \frac{1}{6} + B \right) \pm \frac{1}{2} \sqrt{\frac{1}{4} - \frac{1}{3} B + B^2} \]

6-7

\[ E = -\frac{1}{2} \left( \frac{1}{30} - 3B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} + \frac{1}{5} B + B^2} \]

10-11

\[ E = -\frac{1}{2} \left( \frac{1}{30} - B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} + \frac{1}{15} B + B^2} \]

12-13

\[ E = -\frac{1}{2} \left( \frac{1}{30} + B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} - \frac{1}{15} B + B^2} \]

14-15

\[ E = -\frac{1}{2} \left( \frac{1}{30} + 3B \right) \pm \frac{1}{2} \sqrt{\frac{1}{36} - \frac{1}{5} B + B^2} \]

16-17
10.9.26 Stark Shift in Hydrogen with Fine Structure

Excluding nuclear spin, the \( n = 2 \) spectrum of Hydrogen has the configuration:

\[
\begin{align*}
\Delta E_{FS}/\hbar &= 10 \text{ GHz} \quad \text{(the fine structure splitting)} \\
\Delta E_{Lamb}/\hbar &= 1 \text{ GHz} \quad \text{(the Lamb shift - an effect of quantum fluctuations of the electromagnetic field). These shifts were neglected in the text discussion of the Stark effect. This is valid if } ea_0 E_z >> \Delta E. \end{align*}
\]

Let \( x = ea_0 E_z \).

The diagram above shows the \( n = 2 \) energy levels in Hydrogen including fine structure. We now want to add a Stark effect perturbation \( \hat{H}_{int} = +e\vec{z}E_z \) (corresponds to quantization along \( \vec{E} \)).

We recall the spectroscopic notation \( n\ell_j \). Now for a given \( j \), there are \( 2j + 1 \) degenerate sublevels:

\[
\begin{align*}
2s_{1/2} &\Rightarrow |2s_{1/2}, +1/2 \rangle, |2s_{1/2}, -1/2 \rangle \\
2p_{1/2} &\Rightarrow |2p_{1/2}, +1/2 \rangle, |2p_{1/2}, -1/2 \rangle \\
2p_{3/2} &\Rightarrow |2p_{3/2}, +3/2 \rangle, |2p_{3/2}, +1/2 \rangle, |2p_{3/2}, -1/2 \rangle, |2p_{3/2}, -3/2 \rangle
\end{align*}
\]

Since \( \hat{H}_{int} \) acts only on the spatial degrees of freedom, it is useful to reexpress the eigenstates above in terms of the uncoupled angular momentum basis. This is just standard CG stuff and we have

\[
\begin{align*}
|2s_{1/2}, \pm 1/2 \rangle &= |2s, m_\ell = 0 \rangle \otimes |m_s = \pm 1/2 \rangle \\
|2p_{1/2}, \pm 1/2 \rangle &= \sqrt{\frac{1}{2}} |2p, 0 \rangle \otimes |\pm 1/2 \rangle - \sqrt{\frac{1}{2}} |2p, \pm 1 \rangle \otimes |\mp 1/2 \rangle \\
|2p_{3/2}, \pm 1/2 \rangle &= \sqrt{\frac{1}{2}} |2p, 0 \rangle \otimes |\pm 1/2 \rangle + \sqrt{\frac{1}{2}} |2p, \pm 1 \rangle \otimes |\mp 1/2 \rangle \\
|2p_{3/2}, \pm 3/2 \rangle &= |2p, \pm 1 \rangle \otimes |\pm 1/2 \rangle
\end{align*}
\]

(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.

For weak fields \( ea_0 E_z \leq \Delta E_{Lamb} \), we can restrict our attention to the

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The matrix representation of \( \hat{H}_{\text{int}} \) is block diagonal with no off-diagonal elements between different \( m_j \) as we will see below.

Consider the \( m_j = 1/2 \) 2-dimensional subspace.

\[
\hat{H}_0 + \hat{H}_{\text{int}} = \begin{pmatrix} \Delta E_L & \epsilon \\ \epsilon^* & 0 \end{pmatrix}
\]

where the order of the states labeling the rows and columns is

\[|2s_{1/2}\rangle |2p_{1/2}\rangle\]

and \( \Delta E_L = \) Lamb shift and

\[
\epsilon = \langle 2p_{1/2}, 1/2 | \hat{H}_{\text{int}} | 2s_{1/2}, 1/2 \rangle
\]

To calculate \( \epsilon \), we use the uncoupled representation above:

\[
\epsilon = -eE_z \sqrt{\frac{1}{3}} \langle 2p, 0 | \hat{z} | 2s, 0 \rangle \langle 1/2 | +1/2 \rangle - eE_z \sqrt{\frac{2}{3}} \langle 2p, 1 | \hat{z} | 2s, 0 \rangle \langle -1/2 | +1/2 \rangle
\]

Using \( \langle 2p, 0 | \hat{z} | 2s, 0 \rangle = -a_0 \) as derived in the text, \( \langle 1/2 | +1/2 \rangle = 1 \) and \( \langle -1/2 | +1/2 \rangle = 0 \), we get

\[
\epsilon = -\sqrt{3}e a_0 E_z \) (real)
\]

We diagonalize as follows:

\[
\hat{H} = \begin{pmatrix} \Delta E_L & 0 \\ 0 & 0 \end{pmatrix} + \hat{H}_0 + \hat{H}_{\text{int}} = \epsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

or

\[
\hat{H} = \frac{\Delta E_L}{2} \hat{I} + \frac{\Delta E_L}{2} \hat{\sigma}_z + \epsilon \hat{\sigma}_x
\]

Therefore, the eigenvalues are

\[
E_{\pm} = \frac{\Delta E_L}{2} \pm \sqrt{\frac{(\Delta E_L)^2}{4} + \epsilon^2}
\]

and the eigenvectors are

\[
|\pm\rangle = \cos \left( \frac{\Theta}{2} \right) |2p_{1/2}\rangle \pm \sin \left( \frac{\Theta}{2} \right) |2s_{1/2}\rangle
\]

where

\[
\tan \Theta = \frac{2\epsilon}{\Delta E_L} \) → the so-called mixing angle
Note that this is the ratio of the coupling matrix element to the energy separation.

Thus, the new splitting between the perturbed $2s_{1/2}$ and $2p_{1/2}$ levels is

$$\Delta E'_L = E_+ - E_- = \sqrt{(\Delta E_L)^2 + 4e^2}$$

We need to find the electric field such that $\Delta E'_L = 2\Delta E_L$. We get

$$4e^2 = 3(\Delta E_L)^2 \to \epsilon = \frac{\sqrt{3}}{2} \Delta E_L$$

or

$$\sqrt{3}ea_0 E_z = \frac{\sqrt{3}}{2} \Delta E_L \to E_z = \frac{\Delta E_L}{2ea_0}$$

Now for some numbers. Remember, we are using c.g.s. units. The easiest thing to do is express $\Delta E_L$ in electron volts, so that $\Delta E_L/e$ is in volts. The conversion is via Planck’s constant $h = 4.14 \times 10^{-15}$ eV sec. This gives

$$\Delta E_L = (10^9 \text{Hz})(4.14 \times 10^{-15} \text{eV sec}) = 4.14 \times 10^{-6} \text{eV}$$

Using $a_0 = 0.5 \times 10^{-8} \text{cm (6.5Å)}$ we have

$$E_z = \frac{4.14 \times 10^{-6} \text{V}}{10^{-8} \text{cm}} = 414 \text{V/cm}$$

What about the other substates? There are no off-diagonal matrix elements between different $m_j$.

**PROOF:**

$$\langle 2s_{1/2}, 1/2 | \hat{H}_{int} | 2p_{1/2}, -1/2 \rangle = eE_z \left[ \frac{\sqrt{1}}{3} \langle 2s, 0 | \hat{\vec{z}} | 2p, 0 \rangle \langle 1/2 | -1/2 \rangle - \frac{\sqrt{2}}{3} \langle 2s, 0 | \hat{\vec{z}} | 2p, -1 \rangle \langle 1/2 | 1/2 \rangle \right]$$

Using $\langle 1/2 | -1/2 \rangle = 0$ and $\langle 2s, 0 | \hat{\vec{z}} | 2p, -1 \rangle = 0$ we get

$$\langle 2s_{1/2}, 1/2 | \hat{H}_{int} | 2p_{1/2}, -1/2 \rangle = 0$$

and similarly

$$\langle 2s_{1/2}, -1/2 | \hat{H}_{int} | 2p_{1/2}, 1/2 \rangle = 0$$

The $2 \times 2$ representation for $m_j = -1/2$ is the same as for $m_j = 1/2$.

Thus, in the 4-dimensional subspace of $(2s_{1/2}, 2p_{1/2})$, the representation of $\hat{H}$ is block-diagonal, with two degenerate subblocks

$$\hat{H} = \begin{pmatrix}
\Delta E_L & \epsilon & 0 & 0 \\
\epsilon & 0 & 0 & 0 \\
\ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \Delta E_L & \epsilon \\
0 & 0 & \epsilon & 0
\end{pmatrix}$$
where the top-half corresponds to \( m_j = 1/2 \) and the bottom half to \( m_j = -1/2 \). Thus, the eigenvalues we found earlier are doubly degenerate.

(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 \( 0 \text{GHz} < x < 10 \text{GHz} \).

Comment on the behavior of these curves. Do they have the expected asymptotic behavior? Find analytically the eigenvectors in the limit \( x/\Delta E_{FS} \rightarrow \infty \). Show that these are the expected perturbed states.

We now consider \( ea_0 E_z \geq \Delta E_{FS} \). This means that we must include all of the \( n = 2 \) states.

Again, \( \hat{H} \) is block-diagonal, with no off-diagonal matrix elements between different \( m_j \). These blocks are also doubly degenerate for \( \pm m_j \). There are also \( p \rightarrow p \) matrix elements for parity reasons, i.e., \( \langle 2p, m_j | \hat{z} | 2p, m_j' \rangle = 0 \).

Therefore, we must diagonalize the following \( 3 \times 3 \) matrix

\[
\hat{H} = \begin{pmatrix}
\Delta E_L & \epsilon & \beta \\
\epsilon & 0 & 0 \\
\beta & 0 & \Delta E_{FS}
\end{pmatrix}
\]

where the row/column order is

\[
\begin{pmatrix}
|2s_{1/2}\rangle \\
|2p_{1/2}\rangle \\
|2p_{3/2}\rangle
\end{pmatrix}
\]

Note that \( Ket2p_{3/2}, m_j = \pm 3/2 \) is unperturbed.

We have

\[
\beta = \langle 2p_{3/2}, 1/2 | \hat{H}_{int} | 2s_{1/2}, 1/2 \rangle \\
- eE_z \left[ \frac{\sqrt{2}}{3} \langle 2p, 0 | \hat{z} | 2s, 0 \rangle \langle 1/2 | 1/2 \rangle + \sqrt{\frac{1}{3}} \langle 2p, 1 | \hat{z} | 2s, 0 \rangle \langle -1/2 | 1/2 \rangle \right]
\]

\[
= \sqrt{6}ea_0 E_z
\]

This implies that

\[
\hat{H} = \Delta E_L \begin{pmatrix}
1 & \sqrt{3}x & \sqrt{6}x \\
\sqrt{3}x & 0 & 0 \\
\sqrt{6}x & 0 & 10
\end{pmatrix}
\]

where \( x = ea_0 E_z / \Delta E_L \) and \( \Delta E_L = 1 \text{GHz} \).

Solving for the eigenvalues numerically in the range \( 0 < x < 10 \) we have
Let us now consider the asymptotic behavior. For small $x$ we recover the behavior of part (a) - the level $|2p_{3/2}\rangle$ is too far away to worry about. For sufficiently large $x$, the fine-structure is negligible and we recover the simple linear Stark effect discuss in the text. That we recover the expected eigenvectors can be seen in the large $x$ limit by setting

$$\frac{\Delta E_{FS}}{x} = \frac{\Delta E_L}{x} = 0$$

So that for $x \gg 1$ we get

$$\hat{H} = -x \begin{pmatrix} 0 & \sqrt{3} & \sqrt{6} \\ \sqrt{3} & 0 & 0 \\ \sqrt{6} & 0 & 0 \end{pmatrix}$$

which has eigenvalues $(-3x, 0, 3x)$. That is the linear Stark effect. The eigenvectors (up to an arbitrary overall phase) are

$$|e_1\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} -\sqrt{3} \\ 1 \\ \sqrt{2} \end{pmatrix}$$

$$|e_2\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

$$|e_3\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} \\ 1 \\ \sqrt{2} \end{pmatrix}$$

in the ordered basis

$$|2s_{1/2}\rangle \quad |2p_{1/2}\rangle \quad |2p_{3/2}\rangle \quad m_j = 1/2$$

Therefore, we get

$$|e_1\rangle = \frac{1}{\sqrt{2}}(|2p, 0\rangle - |2s, 0\rangle) \otimes |1/2\rangle$$

$$|e_2\rangle = |2p, 1\rangle \otimes |1/2\rangle$$

$$|e_3\rangle = \frac{1}{\sqrt{2}}(|2p, 0\rangle + |2s, 0\rangle) \otimes |1/2\rangle$$

as expected.

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Note the \( m_j = -1/2 \) are the same asymptotes with \( m_s \rightarrow -m_s \) and the \( m_j = -3/2 \) are flat throughout and yield the remaining states \( |2p, \pm 1 \rangle \otimes |\pm 1/2 \rangle \).

### 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

\[
U(\vec{r}_1 - \vec{r}_2) = C |\vec{r}_1 - \vec{r}_2|^4
\]

using the variational method.

We have

\[
H = \frac{p^2}{2\mu} + V(r)
\]

where \( r = |\vec{r}_1 - \vec{r}_2| \), \( V(r) = Cr^4 \) and \( \mu = m_1 m_2 / (m_1 + m_2) \).

We use a trial function

\[
\psi(\vec{r}) = R(r)Y_{00}(\theta, \phi) = A e^{-\alpha r^2} Y_{00}(\theta, \phi)
\]

Then, normalizing we have

\[
A^2 \int e^{-2\alpha r^2} r^2 dr = 1 \rightarrow A^2 = \frac{4(2\alpha)^{3/2}}{\sqrt{\pi}}
\]

Now

\[
\langle H \rangle = -\frac{\hbar^2}{2\mu} \int R(r) \nabla^2 R(r)r^2 dr + C \int R^2(r)r^6 dr
\]

We have

\[
\nabla^2 R(r) = \frac{1}{r} \frac{\partial}{\partial r} \left( rR(r) \right) = A \frac{1}{r} \frac{\partial}{\partial r} (re^{-\alpha r^2}) = A(4\alpha^2 r^2 - 6\alpha)e^{-\alpha r^2}
\]

Therefore,

\[
\langle H \rangle = -\frac{\hbar^2}{2\mu} A^2 \left[ -6\alpha \int e^{-2\alpha r^2} r^2 dr + 4\alpha^2 \int e^{-2\alpha r^2} r^4 dr \right]
\]

\[
\langle H \rangle = \frac{3 \hbar^2}{2 \mu} \alpha + \frac{15C}{16\alpha^2}
\]

We set

\[
\frac{\partial \langle H \rangle}{\partial \alpha} = 0
\]

to find the value of \( \alpha \) that corresponds to the minimum energy. We have

\[
\frac{\partial \langle H \rangle}{\partial \alpha} = 0 = \frac{3 \hbar^2}{2 \mu} \frac{30C}{16\alpha^3} \rightarrow \alpha^3 = \frac{5 \mu C}{\hbar^2}
\]

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which give an estimated ground state energy of 

$$\langle H \rangle = \frac{3}{2} \frac{\hbar^2}{\mu} \left( \frac{5 \mu C}{\hbar^2} \right)^{1/3} + \frac{15}{16} \left( \frac{5 \mu C}{\hbar^2} \right)^{-2/3} = 2.42 \frac{h^{4/3} C^{1/3}}{\mu^{2/3}}$$

or using a different trial function...

We have

$$H = \frac{p^2}{2\mu} + V(r)$$

where \( r = |\vec{r}_1 - \vec{r}_2| \), \( V(r) = C r^4 \) and \( \mu = m_1 m_2 / (m_1 + m_2) \).

We use a trial function

$$\psi(\vec{r}) = R(r) Y_{00}(\theta, \phi) = Ae^{-\alpha r} Y_{00}(\theta, \phi)$$

Then, normalizing we have

$$A^2 \int e^{-2\alpha r^2} dr = 1 \rightarrow A^2 = 4\alpha^3$$

Now

$$\langle H \rangle = -\frac{\hbar^2}{2\mu} \int R(r) \nabla^2 R(r) r^2 dr + C \int R^2(r) r^6 dr$$

We have

$$\nabla^2 R(r) = \frac{1}{r} \frac{\partial^2}{\partial r^2} (r R(r)) = A \frac{1}{r} \frac{\partial^2}{\partial r^2} (r e^{-\alpha r}) = A \left( \alpha^2 e^{-\alpha r} - \frac{2\alpha}{r} e^{-\alpha r} \right)$$

Therefore,

$$\langle H \rangle = -\frac{\hbar^2}{2\mu} A^2 \left[ -2\alpha \int e^{-2\alpha r} r^4 dr + \alpha^2 \int e^{-2\alpha r} r^2 dr \right]$$

Then

$$\langle H \rangle = \frac{\hbar^2}{2\mu} \alpha^2 + \frac{45C}{2\alpha^3}$$

We set

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0$$

to find the value of \( \alpha \) that corresponds to the minimum energy. We have

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 = \frac{\hbar^2}{\mu} \alpha - \frac{90C}{\alpha^5} \rightarrow \alpha^6 = \frac{90\mu C}{\hbar^2}$$

which give an estimated ground state energy of

$$\langle H \rangle = 2.42 \frac{h^{4/3} C^{1/3}}{\mu^{2/3}}$$

Thus, the Gaussian trial function yields a lower value for \( \langle H \rangle \).
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

\[ \psi_{2s}(\vec{r}) = \frac{1}{\sqrt{4\pi}} \left( \frac{1}{a_0} \right)^{3/2} \left( 2 - \frac{2r}{a_0} \right) e^{-r/a_0} \]

The two-electron wave function must be antisymmetric with respect to interchange of the position and spin variables. Therefore \( S = 0 \rightarrow \) symmetric space function (for the singlet) and \( S = 1 \rightarrow \) antisymmetric space function (for the triplet) or

\[
S = 0 \quad \psi_S(\vec{r}_1, \vec{r}_2) = \frac{\psi_{1s}(\vec{r}_1)\psi_{2s}(\vec{r}_2) + \psi_{1s}(\vec{r}_2)\psi_{2s}(\vec{r}_1)}{\sqrt{2}} \\
S = 1 \quad \psi_T(\vec{r}_1, \vec{r}_2) = \frac{\psi_{1s}(\vec{r}_1)\psi_{2s}(\vec{r}_2) - \psi_{1s}(\vec{r}_2)\psi_{2s}(\vec{r}_1)}{\sqrt{2}}
\]

We let

\[ H = H_0 + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \]

and treat

\[ H' = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \]

as a perturbation.

Now \( \psi_{1s} \) and \( \psi_{2s} \) are both eigenfunctions of \( H_0 \) and the energies of \( \psi_S \) and \( \psi_T \) are equal.

The first-order corrections differ by

\[
\Delta = \langle \psi_S | \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} | \psi_S \rangle - \langle \psi_T | \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} | \psi_T \rangle \\
= 2 \langle \psi_{1s}(\vec{r}_1)\psi_{2s}(\vec{r}_2) | \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} | \psi_{1s}(\vec{r}_2)\psi_{2s}(\vec{r}_1) \rangle \\
= 2 \left( \frac{8}{\pi a_0^3} \right) \left( \frac{1}{4\pi a_0^3} \right) e^2 \int \int d^3r_1 d^3r_2 \left( 2 - \frac{2r_1}{a_0} \right) \left( 2 - \frac{2r_2}{a_0} \right) \frac{e^{-3(r_1 + r_2)/a_0}}{|\vec{r}_1 - \vec{r}_2|}
\]

Now

\[
\frac{1}{|\vec{r}_1 - \vec{r}_2|} = \sum_{\ell} \frac{r_\ell}{r_\ell^{\ell+1}} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell + 1} \frac{Y_{\ell m}(\theta_1, \phi_1) Y_{\ell m}^*(\theta_2, \phi_2)}
\]

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and $e^{-3(r_1 + r_2)/a_0}$ is invariant under separate rotation of the $\vec{r}_1$ and $\vec{r}_2$. Therefore, only the $\ell = 0$ term survives the angular integration. We then have

$$\Delta = 2(4\pi)^2 \left( \frac{8}{\pi a_0^3} \right) \left( \frac{1}{4\pi a_0^3} \right) e^2 \int_0^\infty r_1^2 dr_1 \left( 2 - \frac{2r_1}{a_0} \right) e^{-3r_1/a_0} \int_0^\infty r_2^2 dr_2 \left( 2 - \frac{2r_2}{a_0} \right) e^{-3r_2/a_0} \frac{1}{r_2}$$

$$= \frac{128\pi^2}{a_0^6} \int_0^\infty r_1^2 dr_1 \left( 2 - \frac{2r_1}{a_0} \right) e^{-3r_1/a_0} \int_0^\infty r_2^2 dr_2 \left( 2 - \frac{2r_2}{a_0} \right) e^{-3r_2/a_0} \frac{1}{r_2}$$

$$= \frac{64}{729} a_0 = 2.39 \text{ eV}$$

10.9.29 Hyperfine Interaction in the Hydrogen Atom

Consider the interaction

$$H_{hf} = \mu_B \mu_N \frac{\vec{S}_1 \cdot \vec{S}_2}{a_B^3} \hbar^2$$

where $\mu_B$, $\mu_N$ 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:

$$E_t = -1 \text{ Ry} + \frac{A}{4}, \quad E_s = -1 \text{ Ry} - \frac{3A}{4}$$

and that the corresponding states are triplets and singlets, respectively.

Instead of the $|S, m_1, S_2, m_2\rangle$ basis ($|m_1, m_2\rangle = |++, |+\mp, |\pm\pm, |\mp\mp\rangle$), use the total spin ($\text{total } J$) basis $|S m\rangle = |1, 1\rangle, |1, 0\rangle, |1, -1\rangle, |0, 0\rangle$.

Then rewrite $\vec{S}_1 \cdot \vec{S}_2$ in terms of the total spin $\vec{S}$:

$$\vec{S}^2 = (\vec{S}_1 + \vec{S}_2)^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2\vec{S}_1 \cdot \vec{S}_2$$

For electron and proton,

$$S_1 = \frac{1}{2} = S_2$$

so that

$$\vec{S}_1^2 \rightarrow \hbar^2 \left( \frac{1}{2} \right) \left( \frac{1}{2} + 1 \right) = \frac{3}{4} \hbar^2 = S_2^2$$

Both of these operators are simply constants (i.e., times the identity) throughout this Hilbert space.

We get the allowed $S$ values by

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1 \rightarrow S = 0, 1$$

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and in the \(|Sm\rangle\) basis: \(\vec{S}^2 \rightarrow \hbar^2 S(S + 1)\) which equals 0 for the singlet \(S = 0\) and \(2\hbar^2\) for the triplet \(S = 1\). Therefore in the singlet

\[
S = 0 \quad \vec{S}_1 \cdot \vec{S}_2 = -\frac{3}{4} \hbar^2
\]

and in the triplet

\[
S = 1 \quad \vec{S}_1 \cdot \vec{S}_2 = \frac{1}{4} \hbar^2
\]

The energy before considering \(H_{hf}\) is \(-1\) Ry. \(H_{hf}\) splits these into

\[
S = 1 \quad \text{triplet} \quad E_t = -1 \text{ Ry} + \frac{A}{4}
\]

\[
S = 0 \quad \text{singlet} \quad E_s = -1 \text{ Ry} - \frac{3A}{4}
\]

where

\[
A = \frac{\mu_B \mu_N}{a_B^2}
\]

(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.

We have

Separation is \(A = \frac{\mu_B \mu_N}{a_B^2} = \mu_B = g_e \frac{e\hbar}{2mc} (g_e = 2), \mu_N = g_N \frac{e\hbar}{2Mc} (g_N = 5.6)\)

Therefore,

\[
A = g_e g_N \frac{e^2\hbar^2}{a_B^2 4mMc^2} = 11.2 \times \frac{e^2\hbar^2}{a_B^2 4mMc^2}
\]

Now

\[
\frac{e^2\hbar^2}{a_B^2 4mMc^2} = \frac{mc^2}{\hbar} \frac{e^2}{a_B} \approx 0.18 \times 10^{-6} \text{ eV}
\]

Thus the splitting is \(A = 2.09 \times 10^{-6} \text{ eV}\). Now \(1 \text{ eV} \leftrightarrow \lambda = 1.24 \times 10^4 \text{ cm}\). Therefore this splitting corresponds to

\[
\lambda_{hf} = \frac{1.24 \times 10^4}{2.09 \times 10^{-6}} = 59.3 \text{ cm}
\]

We note that the dipole-dipole interaction that was implied in stating this problem, actually vanishes for a (spherical) \(s\) state due to the angular dependence. However, in the hydrogen atom there is another contribution to the energy that depends on the relative spin orientation of the electron and proton and therefore has the form \(BS_1 \cdot S_2\). This is the contact hyperfine interaction, due to the electron density at the proton.
site $|\psi(0)|^2 = 1/(a_0^3)$. Remarkably, because of this $1/a_0^3$ dependence the prefactor $B$ is of the same order of magnitude as that of the dipole-dipole interaction. In the text we show that the correct hyperfine splitting is

$$\Delta E = \frac{4g_p^4 \hbar^4}{3M_p m_e^2 c^2 a_0^3} = 5.88 \times 10^{-6} \text{eV}$$

which in frequency is $\nu = 1420 \text{MHz}$, and in wavelength is $21 \text{cm}$ - the famous $21 \text{cm}$ line seen in spectra emanating from interstellar space.

### 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).

First, the general approach. The idea is to express everything in angular momentum language which does a lot of the algebra for you. It is a tiny bit of algebra to convert the vector $\vec{d}$ to the spherical tensor $d_1^q$. It is a similar tiny amount of work to find appropriate linear combination of the spherical harmonics. But, when this is done, what is left is to evaluate nine matrix elements, which with the help of the Wigner-Eckhart theorem works like this:

$$\langle 100|d_1^q|2im\rangle \rightarrow \langle 10||d||21\rangle \langle 00|1q;1m\rangle$$

(The principal quantum number $n$ has been made boldface to distinguish it from the angular momentum indices). The first quantity is the reduced matrix element which is one radial integral (independent of $q$ and $m$), and the rst is the CG coefficient. For the CG coefficients, one can check their selection rules to see that a lot of them vanish, then look up the rest. I will outline the main steps below(some of the lines might be a little rough, but the process will be clear.

(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-Gordan coefficients.

First, convert $\vec{d} \leftrightarrow d_1^q$. We have

$$d_1^0 = d_z \quad , \quad d_1^{\pm 1} = \mp \frac{1}{\sqrt{2}}(d_x \pm id_y)$$
We then have for the $p_x, p_y, p_z$ orbitals

$$\psi_{210} = C \frac{r}{a_0} e^{-r/2a_0} \cos \theta \equiv p_z \quad C = \left( \frac{1}{32\pi a_0^3} \right)^{1/2}$$

$$\psi_{21+1} = \frac{C}{\sqrt{2} a_0} \frac{r}{a_0} e^{-r/2a_0} \sin \theta e^{\pm i\phi}$$

$$\equiv \frac{C}{a_0} e^{-r/2a_0} \left( \sin \theta \left( \cos \phi \pm i \sin \phi \right) \right) \equiv \mp p_x \pm ip_y$$

We then have

$$p_x = \frac{1}{\sqrt{2}} (-\psi_{211} + \psi_{21-1}) \quad p_y = -i \frac{1}{\sqrt{2}} (\psi_{211} + \psi_{21-1})$$

(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 $(\ell, m)$ indices).

Normalizing properly we have

$$\psi_{210} = R_{21}(r) Y_{10}, \quad Y_{10} = \sqrt{\frac{3}{4\pi}} \cos \theta$$

so that

$$\psi_{210} = \sqrt{\frac{3}{4\pi}} C \left( \sqrt{\frac{3}{4\pi}} \cos \theta \right) \frac{r}{a_0} e^{-r/2a_0}$$

and thus

$$R_{21}(r) = \frac{1}{(24a_0^3)^{1/2}} \frac{r}{a_0} e^{-r/2a_0}$$

and therefore

$$\psi_{21m} = R_{21}(r) Y_{1m}(\theta, \phi)$$

We then have

$$\langle 1s | \hat{d} | 2p_x \rangle = \left( \int R_{1s}^* (-e r) R_{2p} r^2 dr \right) \langle Y_{00} | \hat{d} | 2p_x \rangle$$

The value of the radial integral is

$$\int R_{1s}^* (-e r) R_{2p} r^2 dr = -\frac{4!}{\sqrt{6}} \left( \frac{2}{3} \right)^5 ea_0$$

(c) Reconstruct the vector matrix elements.

$$\langle 1s | \hat{d} | 2p_j \rangle$$

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and discuss the angular dependence you find.

Putting things together, the result is , using

\[ D = -\frac{4!}{\sqrt{6}} \left(\frac{2}{3}\right)^5 e a_0 \]

\[ \langle 1s | \vec{d} | 2p_x \rangle = (D, 0, 0), \quad \langle 1s | \vec{d} | 2p_y \rangle = (0, D, 0), \quad \langle 1s | \vec{d} | 2p_z \rangle = (0, 0, D) \]

You should have guessed that the one involving \( p_y \) would look a lot like the one for \( p_x \) except being rotated \( x \to y \) some way .... and also for \( z \).

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 \( \psi_\alpha(x) = e^{-\alpha x^2} \). Show that the variational approach gives the exact ground state energy.

Using the Gaussian trial function

\[ \psi_\alpha(x) = e^{-\alpha x^2} \]

we have the mean energy

\[ \bar{H}_\alpha = \frac{\langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle} \]

Now

\[ \langle \psi_\alpha | \psi_\alpha \rangle = \int_{-\infty}^{\infty} dx e^{-2\alpha x^2} = \sqrt{\frac{\pi}{2\alpha}} \]

and

\[ \langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle = \int_{-\infty}^{\infty} dx \psi_\alpha(x) \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) \psi_\alpha(x) \]

\[ = \frac{\hbar^2}{2m} \sqrt{\frac{\pi}{2\alpha}} + \frac{1}{8} m \omega^2 \sqrt{\frac{\pi}{2\alpha^3}} \]

Therefore,

\[ \bar{H}_\alpha = \frac{\hbar^2}{2m} \alpha + \frac{1}{8} m \omega^2 \frac{1}{\alpha} \]

Then we have

\[ \frac{d\bar{H}_\alpha}{d\alpha} = 0 \Rightarrow \frac{\hbar^2}{2m} - \frac{1}{8} m \omega^2 \frac{1}{\alpha^2} \]

or

\[ \alpha_{min} = \frac{m \omega}{2\hbar} \]
Thus,
\[ \psi_{\alpha_{\text{min}}}(x) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-m\omega x^2/2\hbar}, \quad \bar{H}_{\text{min}} = \frac{\hbar\omega}{2} \]
which is the correct ground state energy and wave function! The moral here is: if, by chance you choose the exact from of the trial ground state, minimization of the mean energy will lead to an exact solution.

(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? We now have as above
\[ \langle \psi_\alpha | \psi_\alpha \rangle = \frac{\pi}{2\alpha^{3/2}} \]
and
\[ \langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle = \frac{\pi\hbar^2}{8m\alpha^{5/2}} + \frac{\pi}{4} m\omega^2 \alpha^{-1/2} \]
so that
\[ \bar{H}_\alpha = \frac{\hbar^2}{2m\alpha} + \frac{1}{2} m\omega^2 \alpha \]
Now
\[ \frac{d\bar{H}_\alpha}{d\alpha} = 0 \rightarrow \alpha_{\text{min}} = \frac{\hbar}{\sqrt{2m\omega}} \]
and therefore
\[ \bar{H}_{\text{min}} = \frac{\hbar\omega}{\sqrt{2}} \]
This is not bad! It is 20% of \( \hbar \omega \) off from the exact answer. Although the variational method can give reasonably close answers for the ground state energy, it is not a controlled approximation, i.e., there is no small parameter with which we can know the accuracy of the result.

(c) Now consider the double oscillator with potential
\[ V(x) = \frac{1}{2} m\omega^2(|x| - a)^2 \]
as shown below:
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.

Since \( V(x) \) is invariant under reflection, the eigenstates have good parity, i.e., they are symmetric or antisymmetric. Therefore, we choose
\[ \psi_n^{(\pm)}(x) = u_n(x - a) \pm u_n(x + a) \]

where \( u_n(x) \) is the harmonic oscillator wave function (Hermite polynomial \( \times \) Gaussian.

(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
\[
A_n = \int u_n(x - a) \hat{H} u_n(x - a) dx \\
B_n = \int u_n(x - a) \hat{H} u_n(x + a) dx \\
C_n = \int u_n(x + a) \hat{H} u_n(x - a) dx
\]

In this case, the variational estimate is the mean value since we have no parameter to minimize. Thus,
\[ E_n^{(\pm)} = \frac{\langle \psi_n^{(\pm)} | \hat{H} | \psi_n^{(\pm)} \rangle}{\langle \psi_n^{(\pm)} | \psi_n^{(\pm)} \rangle} \]
Now
\[ \langle \psi_n^{(\pm)} | \psi_n^{(\pm)} \rangle = \langle u_n^{(+)} | u_n^{(+)} \rangle + \langle u_n^{(-)} | u_n^{(-)} \rangle + 2 \langle u_n^{(+)} | u_n^{(-)} \rangle = 1 + 2 + 2C_n \]

where \( u_n^{(\pm)} = u_n(x \mp a) = \langle x | u_n^{(\pm)} \rangle \) and
\[ \langle \psi_n^{(\pm)} | \hat{H} | \psi_n^{(\pm)} \rangle = \langle u_n^{(+)} | \hat{H} | u_n^{(+)} \rangle + \langle u_n^{(-)} | \hat{H} | u_n^{(-)} \rangle \]
\[ \pm \langle u_n^{(+)} | \hat{H} | u_n^{(-)} \rangle \pm \langle u_n^{(-)} | \hat{H} | u_n^{(+)} \rangle \]
\[ = 2(A_n \pm B_n) \text{ by parity} \]

Therefore
\[ E_n^{\pm} = \frac{A_n \pm B_n}{1 + C_n} \]

(c) 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 \( V_0 = m\omega^2a^2/2 \). This is known as the ground tunneling splitting. Explain why?

For the ground state
\[ u_0(x) = \left( \frac{\beta}{\pi} \right)^{1/4} e^{-\beta x^2/2}, \quad \beta = \frac{m\omega \hbar}{\hbar} \]

The ground state splitting is
\[ \Delta E_0 = E_0^{(-)} - E_0^{(+)} = -\frac{2B_0}{1 + C_0} \]

where
\[ C_0 = \int_{-\infty}^{\infty} dx u_0(x + a) u_0(x - a) = \sqrt{\frac{\beta}{\pi}} \int_{-\infty}^{\infty} dx e^{-\beta(x+a)^2+(x-a)^2}/2 \]
\[ = e^{-\beta a^2} \sqrt{\frac{\beta}{\pi}} \int_{-\infty}^{\infty} dx e^{-\beta x^2} = e^{-\beta a^2} \]

and
\[ B_0 = \int_{-\infty}^{\infty} dx u_0(x + a) \hat{H} u_0(x - a) = \int_{-\infty}^{0} dx u_0(x + a) \hat{H} u_0(x - a) \]
\[ + \int_{0}^{\infty} dx u_0(x + a) \hat{H} u_0(x - a) \]
where
\[ \hat{H}_\pm = \hat{p}^2/2m + \frac{1}{2}m \omega^2(x \mp a)^2 \]

We note that the eigenvalue equations are
\[ \hat{H}_\pm u_0(x \mp a) = \frac{\hbar \omega}{2} u_0(x \mp a) \]

Aside: we have
\[ \int_{-\infty}^{0} dx u_0(x + a) \hat{H}_- u_0(x - a) = \int_{-\infty}^{0} dx \left( \hat{H}_- u_0(x + a) \right) u_0(x - a) \]

where we have used integration by parts. We then get
\[ B_0 = \frac{\hbar \omega}{2} \left( 1 - 2 \sqrt{\frac{\beta}{\pi}} a \right) e^{-\beta a^2} \]

which implies that
\[ \Delta E_0 = \hbar \omega \left( 1 - 2 \sqrt{\frac{\beta}{\pi}} a \right) \frac{e^{-\beta a^2}}{1 + e^{-\beta a^2}} \]

For \( a \gg \sqrt{\hbar/m \omega} \), this gives
\[ \Delta E_0 = 2\hbar \omega \sqrt{\frac{\beta}{\pi}} a e^{-\beta a^2} \]

Noting that
\[ \beta a^2 = \frac{m \omega a^2}{\hbar} = \frac{2V_0}{\hbar} \]

so that
\[ \Delta E_0 = 2\hbar \omega \sqrt{\frac{2V_0}{\hbar \omega}} ae^{-2V_0/\hbar \omega} \]

This is known as the \textit{tunneling splitting} since the energy difference determines the frequency of tunneling between the left/right wells, i.e., \( \omega_{\text{tunnel}} = \Delta E_0/\hbar \).

(f) This approximation clearly breaks down as \( a \to 0 \). Think about the limits and sketch the energy spectrum as a function of \( a \).

When \( a \gg \sqrt{\hbar/m \omega} \), we have tunneling splitting. When \( a \to 0 \) we have a single oscillator: \( \hbar \omega(n + 1/2) \). The ground-sate doublet is as shown below
The symmetric state must match onto the ground state of the single oscillator.

The antisymmetric state must match on to the first excited state. This is shown below.

\[ \psi(x) = (x - a)(x + a) \]

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 \( \psi'' \) at \( x = \pm a \) do not contribute to the energy.

We have

\[ \psi(x) = \begin{cases} 0 & x < -a \\
(x - a)(x + a) & -a < x < a \\
0 & x > a \end{cases} \]

The Hamiltonian (inside the well) is

\[ H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \]
Thus,

\[ E_0 \leq \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{-\frac{\hbar^2}{2m} \int_a^{-a} dx (x-a)(x+a) \frac{d^2}{dx^2} (x-a)(x+a)}{\int_a^{-a} dx (x-a)^2(x+a)^2} \]

\[ E_0 \leq \frac{-\frac{\hbar^2}{2m} \int a^{-a} dx (x^2-a^2)}{\int_a^{-a} dx (x^2-a^2)^2} = \frac{-\frac{\hbar^2}{m} \left[ \frac{x^3}{3} - a^2 x \right]_a^{-a}}{\left[ \frac{x^5}{5} - 2a^2 x^3 + a^4 x \right]_a^{-a}} = \frac{\hbar^2}{m} \frac{4a^3}{15a^5} \]

\[ E_0 \leq \frac{5}{4ma} \frac{\hbar^2}{ma^2} = 1.25 \frac{\hbar^2}{ma^2} \]

The exact solution gives the result

\[ E_{0,\text{exact}} = \frac{\pi^2}{8} \frac{\hbar^2}{ma^2} = 1.2325 \frac{\hbar^2}{ma^2} \]

so \( E_{0,\text{exact}} \leq E_0 \) as expected.

**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 \(-ma^2V_0^2/2\hbar^2\).

For \( V(x) = -aV_0 \delta(x) \) and the Gaussian trial function \( \psi = e^{-\alpha x^2} \) we have

\[ E_0 \leq \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{-\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx e^{-\alpha x^2} \frac{d^2}{dx^2} e^{-\alpha x^2} - aV_0 \int_{-\infty}^{\infty} dx e^{-2\alpha x^2} \delta(x)}{\int_{-\infty}^{\infty} dx e^{-2\alpha x^2}} \]

\[ E_0 \leq \frac{-\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx e^{-2\alpha x^2} (4\alpha^2 x^2 - 2\alpha) - aV_0}{\int_{-\alpha}^{\alpha} \sqrt{\frac{2\alpha}{\pi}}} = \frac{-\frac{\hbar^2}{2m} \left( \left( \frac{4\alpha^2}{2(2\alpha)^{3/2}} \right) - 2\alpha \right) - aV_0}{\sqrt{\frac{2\alpha}{\pi}}} \]

\[ E_0 \leq -\sqrt{\frac{2\alpha}{\pi}} \left( aV_0 + \frac{\hbar^2}{2m} \left( \frac{1}{\sqrt{2}} \alpha^{1/2} \sqrt{\pi} - \sqrt{2} \alpha^{1/2} \sqrt{\pi} \right) \right) = -\sqrt{\frac{2\alpha}{\pi}} \left( aV_0 + \frac{\hbar^2}{2m} \alpha^{1/2} \sqrt{\pi} \left( \frac{1}{\sqrt{2}} - \sqrt{2} \right) \right) \]

Now,

\[ \frac{dE_0}{d\alpha} = 0 \rightarrow -\sqrt{\frac{2\alpha}{\pi}} \left( \frac{1}{2} aV_0 \alpha^{-1/2} + \frac{\hbar^2}{2m} \sqrt{\pi} \left( \frac{1}{\sqrt{2}} - \sqrt{2} \right) \right) \]

\[ \alpha^{1/2} = \frac{aV_0}{\frac{\hbar^2}{2m} \sqrt{\pi} \left( \frac{1}{\sqrt{2}} - \sqrt{2} \right)} = \frac{maV_0 \sqrt{2}}{\hbar \sqrt{\pi}} \]

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so that
\[
E_0 \leq -\sqrt{\frac{2\alpha}{\pi}} \left( aV_0 + \frac{\hbar^2}{2m} a^{1/2} \sqrt{\pi} \left( \frac{1}{\sqrt{2}} - \sqrt{2} \right) \right) = -\frac{maV_0}{\hbar^2 c} \sqrt{\frac{2}{\pi}} \left( aV_0 - \frac{\hbar^2}{2m \hbar^2 c} \sqrt{\pi} \right) \]
\[
E_0 \leq -\frac{ma^2 V_0^2}{\pi \hbar^2} = -0.318 \frac{ma^2 V_0^2}{\pi \hbar^2} \]

The exact result is
\[
E_{0, \text{exact}} = -0.500 \frac{ma^2 V_0^2}{\hbar^2} < E_0 \]
as expected.

### 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 \( \hbar \omega/2 \).

We use the trial function
\[
\psi(x) = \begin{cases} 
x^4 - 2a^2x^2 + a^4 & |x| \leq a \\
0 & |x| > a 
\end{cases}
\]
for a harmonic oscillator Hamiltonian where \( V(x) = m\omega^2 x^2/2 \). Now we have
\[
\int_{-a}^{a} \psi^* \psi dx = 0.81a^9 \\
\int_{-a}^{a} \psi^* V(x) \psi dx = 0.70ma^2 \omega a^11 \\
-\frac{\hbar^2}{2m} a^7 \int_{-a}^{a} \psi^* \frac{d^2}{dx^2} \psi dx = 1.23 \frac{\hbar^2}{2m} a^7 
\]
Therefore,
\[
E_0 \leq \frac{1.23 \frac{\hbar^2}{2m} a^7 + 0.70ma^2 \omega a^{11}}{0.81a^9} = 1.52 \frac{\hbar^2}{ma^2} + 0.86ma^2 \omega a^2 
\]
Minimizing, we have
\[
\frac{dE_0}{da} = 0 \rightarrow a^2 = 1.33 \frac{\hbar}{m\omega} 
\]
so that
\[
E_0 \leq 2.28\hbar \omega 
\]
The exact answer is
\[
E_{0, \text{exact}} = 0.50\hbar \omega < E_0 
\]as expected.
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 \( m = \text{mass}, \, \hbar \) and \( g \).

The Schrödinger equation is

\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + g \, |x| \right) \psi(x) = E \psi(x) \rightarrow \left( \frac{d^2}{dx^2} + \frac{2m}{\hbar^2} (E - g \, |x|) \right) \psi(x) = 0
\]

Since

\[
\left[ \frac{mE}{\hbar^2} \right] = L^{-2} \quad \text{and} \quad \left[ \frac{mg}{\hbar^2} \right] = L^{-3} \rightarrow \left[ \frac{mE}{\hbar^2} \right]^3 \leftrightarrow \left[ \frac{mg}{\hbar^2} \right]^2 \rightarrow E \propto \left( \frac{h^2}{m^2 g^2} \right)^{1/3}
\]

or the eigenvalues have the form

\[
E_n = \left( \frac{h^2}{m^2 g^2} \right)^{1/3} f(n)
\]

where \( f(n) \) is a function of a positive integer \( n \).

(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.

We first normalize the trial function

\[
\psi(x) = c \theta(x + a) \theta(a - x) \left( 1 - \frac{|x|}{a} \right)
\]

We have

\[
1 = \int \psi^*(x) \psi(x) dx = |c|^2 \int \left( \theta(x + a) \theta(a - x) \left( 1 - \frac{|x|}{a} \right) \right)^2 dx
\]

\[
= |c|^2 \int_{-a}^{a} \left( 1 - \frac{|x|}{a} \right)^2 dx = \frac{2a}{3} |c|^2 \rightarrow |c|^2 = \frac{3}{2a}
\]

We then calculate the expectation value of \( \hat{H} \) using the trial function

\[
\langle \hat{H} \rangle = \int \psi^*(x) \hat{H} \psi(x) dx = \int \psi^*(x) \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + g \, |x| \right) \psi(x) dx
\]

\[
= -\frac{\hbar^2}{2m} \int \psi^*(x) \frac{d^2 \psi(x)}{dx^2} dx + g \int \psi^*(x) |x| \psi(x) dx
\]
Now,
\[ \int \psi^*(x) |x| \psi(x) dx = |c|^2 \left( - \int_{-a}^0 x \left( 1 + \frac{x}{a} \right)^2 dx + \int_a^q x \left( 1 - \frac{x}{a} \right)^2 dx \right) = \frac{a^2}{b} |c|^2 = \frac{a}{4} \]
and
\[ \frac{d\psi}{dx} = c \delta(x+a) \theta(a-x) \left( 1 - \frac{|x|}{a} \right) - c \theta(x+a) \delta(a-x) \left( 1 - \frac{|x|}{a} \right) + c \theta(x+a) \theta(a-x) \left( - \frac{|x|}{x} \right) \]
Therefore, we have
\[ \int \psi(x) \frac{d^2 \psi(x)}{dx^2} dx = \psi(x) \frac{d\psi(x)}{dx} \bigg|_{-\infty}^{\infty} - \int_{-\infty}^{-\infty} \left( \frac{d\psi(x)}{dx} \right)^2 dx = - \int_{-\infty}^{-\infty} \left( \frac{d\psi(x)}{dx} \right)^2 dx \]
and thus
\[ \langle H \rangle = \frac{3h^2}{2ma^2} + \frac{g a}{4} \]
For its minimum value we have
\[ \frac{d}{da} \langle H \rangle = 0 = - \frac{3h^2}{ma^3} + \frac{g}{4} \rightarrow a = \left( \frac{12h^2}{4mg} \right)^{1/3} \]
so that the estimate of the ground state energy is
\[ \langle H \rangle = \frac{3h^2}{2m \left( \frac{12h^2}{4mg} \right)^{2/3}} + \frac{g \left( \frac{12h^2}{4mg} \right)^{1/3}}{4} = \frac{3}{4} \left( \frac{3h^2 g^2}{2m} \right)^{1/3} \]
(c) Why is the trial function \( \psi(x) = c \theta(x+a) \theta(a-x) \) not a good one?
If we had used the trial function
\[ \psi(x) = c \theta(x+a) \theta(a-x) \]
and repeated the above calculation we would get
\[ 1 = \int \psi^*(x) \psi(x) dx = 2a |c|^2 \rightarrow |c|^2 = \frac{1}{2a} \]
\[ \int \psi(x) \frac{d^2 \psi(x)}{dx^2} dx = 0 \]
\[ \int \psi^*(x) |x| \psi(x) dx = a^2 |c|^2 = \frac{a}{2} \]
so that
\[ \langle H \rangle = \frac{ga}{2} \rightarrow \frac{d}{da} \langle H \rangle = 0 = \frac{g}{2} \neq 0 \]
that is, \( \langle H \rangle \) has no extremum, Therefore, the trial function is not good.
(d) Describe briefly (no equations) how you would go about finding a variational estimate of the energy of the first excited state.

We first choose a trial function for the 1st excited state that is orthogonal to the ground state. Then we use the same method as above.

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.

\( H_0 \) commutes with \( L^2 \), \( S^2 \), and \( J^2 \) and common eigenstates can be found. The eigenvalues of \( H_0 \) can depend on \( \ell \), but not on \( s \) and \( j \).

We denote the common eigenbasis of \( H_0 \), \( L^2 \), \( S^2 \), and \( J^2 \) by \( \{|n\ell s; jm_j\}\} \).

The first-order energy correction due to the perturbation is

\[ \langle H' \rangle_{n\ell j} = \langle n\ell s; jm_j | H' | n\ell s; jm_j \rangle \]

Now

\[ \vec{S} \cdot \vec{L} = \frac{1}{2} (J^2 - L^2 - S^2) \]

Therefore

\[ \langle H' \rangle_{n\ell j} = \frac{1}{2} A(j(j + 1) - \ell(\ell + 1) - s(s + 1)) \]

which is independent of \( m_j \). Now the possible values of \( j \) are \( j = \ell \pm 1/2 \) and there are \( 2j + 1 \) terms for each \( j \).

The average perturbation is

\[ (2(\ell + 1/2) + 1) \frac{1}{2} A((\ell + 1/2)(\ell + 3/2) - \ell(\ell + 1) - 3/4) \]

\[ + (2(\ell - 1/2) + 1) \frac{1}{2} A((\ell - 1/2)(\ell + 1/2) - \ell(\ell + 1) - 3/4) \]

\[ = A\ell^2 + A\ell - A\ell - A\ell^2 = 0 \]
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.

We have a system where

\[ \hat{H}_0 = \frac{\vec{p}^2}{2m} + \frac{1}{2} m \omega^2 r^2 \rightarrow \text{3-dimensional harmonic oscillator} \]

and

\[ V = \lambda \vec{\sigma} \cdot \vec{r} \]

is a perturbation.

The unperturbed ground state is 2-fold degenerate (spin-up and spin-down along the \( z \)-axis).

Unperturbed states:

\[ |n_x n_y n_z; \pm \rangle \rightarrow E^{(0)}_{n_x n_y n_z} = (n_x + n_y + n_z + 3/2) \hbar \omega \]

ground - state \( \rightarrow n_x = n_y = n_z = 0 \)

Now since \( E^{(1)}_1 = \langle 000; \pm | V | 000; \pm \rangle = 0 \) the first-order energy correction is zero and the states are still degenerate to first-order.

Therefore, we must apply second-order degenerate perturbation theory. We get

\[ 0 = \det \left| \sum_{m \neq |000; \pm \rangle} V_{000 \pm m} V_{m,000} \frac{E^{(0)}_{m00} - E^{(0)}_{000}}{E^{(0)}_{m00} - E^{(0)}_{000}} - E \right| \]

To evaluate this expression we need the matrix elements

\[ \lambda \langle 000; \pm | \vec{\sigma} \cdot \vec{r} | m \rangle = \lambda \langle 000; \pm | (\hat{\sigma}_x x + \hat{\sigma}_y y + \hat{\sigma}_z z) | n_x n_y n_z; s_z \rangle \]

the only nonzero terms come from

\[ \lambda \langle 000; \pm | (\hat{\sigma}_x x | 100; \mp \rangle \]

or

\[ \lambda \langle 000; \pm | (\hat{\sigma}_y y) | 010; \mp \rangle \]

or

\[ \lambda \langle 000; \pm | (\hat{\sigma}_z z) | 001; \pm \rangle \]

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so we have only six nonzero contributions. In all these cases
\[ E^{(0)}_{000} - E^{(0)}_m = \frac{3}{2} \hbar \omega - \frac{5}{2} \hbar \omega = -\hbar \omega \]

Now
\[ \langle 0 | x | 1 \rangle = \langle 0 | y | 1 \rangle = \langle 0 | z | 1 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \]

and
\[ \langle \pm | \hat{\sigma}_x | \mp \rangle = 1, \quad \langle \pm | \hat{\sigma}_y | \mp \rangle = \mp i, \quad \langle \pm | \hat{\sigma}_z | \pm \rangle = \pm 1 \]

Therefore,
\[ \sum_{m \neq |000;\pm\rangle} \frac{V_{000+m}V_{m,000}}{E^{(0)}_{000} - E^{(0)}_m} - \frac{\lambda^2}{h\omega} (1 + 1 + 1) \frac{\hbar}{2m\omega} = -\frac{3\lambda^2}{2m\omega^2} = \sum_{m \neq |000;\pm\rangle} \frac{V_{000-m}V_{m,000-}}{E^{(0)}_{000} - E^{(0)}_m} \]
\[ \sum_{m \neq |000;\pm\rangle} \frac{V_{000+m}V_{m,000-}}{E^{(0)}_{000} - E^{(0)}_m} \]

We get a diagonal result so that the degeneracy remains to second-order and we have
\[ E_{000} = \frac{3}{2} \frac{\omega}{\hbar} - \frac{3\lambda^2}{2m\omega^2} \]

10.9.38 Interacting with the Surface of Liquid Helium

An electron at a distance \( x \) from a liquid helium surface feels a potential
\[ V(x) = \begin{cases} -K/x & x > 0 \\ \infty & x \leq 0 \end{cases} \]

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.

For \( x \leq 0 \), the wave function \( \psi(x) = 0 \) and for \( x > 0 \) the Schrödinger equation is
\[ \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \frac{K}{x} \right) \psi(x) = E\psi(x) \]

For a hydrogen atom, the radial wave function satisfies the equation
\[ \left( \frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) + \frac{\ell(\ell + 1)\hbar^2}{2mr^2} - \frac{e^2}{r} \right) R(r) = ER(r) \]
Letting \( R(r) = \frac{\chi(r)}{r} \), \( \ell = 0 \) we get

\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} - \frac{e^2}{r} \right) \chi(r) = E\chi(r)
\]

which, mathematically is the same equation as above. The boundary conditions in both case are identical. Therefore, the solutions must be the same with the substitutions

\[ r \leftrightarrow x \quad , \quad e^2 \leftrightarrow K \]

so that the hydrogen solutions

\[ E_{10} = -\frac{m e^4}{2\hbar^2} \quad , \quad \chi_{10}(r) = \frac{2r}{a_0^{3/2}} e^{-r/a_0} \quad , \quad a_0 = \frac{\hbar^2}{m e^2} \]

become

\[ E^{(0)}_1 = -\frac{m K^2}{2\hbar^2} \quad , \quad \psi^{(0)}_1(x) = \frac{2x}{a^{3/2}} e^{-x/a} \quad , \quad a = \frac{\hbar^2}{m K} \]

An electric field in the \( x \)-direction gives a perturbation \( V = e\varepsilon x \) so that the energy correction to the ground state in first-order is

\[ E^{(1)}_1 = \left\langle \psi^{(0)}_1 \right| V \left| \psi^{(0)}_1 \right\rangle = \frac{4e\varepsilon}{a^3} \int_0^\infty x^3 e^{-2x/a} dx = \frac{3}{2} e\varepsilon a = \frac{3e\varepsilon \hbar^2}{2m K} \]

### 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.

By analogy with the hydrogen atom, the normalized wave function for the 1s ground state of positronium is

\[ \psi_{100}(\vec{r}) = \frac{1}{\sqrt{\pi}} \left( \frac{1}{2a_0} \right)^{3/2} e^{-r/2a_0} \quad , \quad a_0 = \frac{\hbar^2}{m e^2} \]

Note that the factor of 2 in the exponential is to account for the fact that the reduced mass is \( \mu = m/2 \).

(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?
The mean square radius for the $1s$ state is

$$\langle r^2 \rangle = \frac{1}{8\pi a_0^3} \int_0^\infty e^{-r/a_0} r^4 dr = \frac{a_0^3}{8\pi} \int_0^\infty e^{-z} z^4 dx = \frac{3a_0^3}{\pi}$$

Therefore, the root-mean-square radius is

$$\sqrt{\langle r^2 \rangle} = \sqrt{\frac{3}{\pi} a_0}$$

This is a reasonable estimate of the 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

$$\vec{\mu} = \frac{ge}{2mc} \vec{S}$$

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!

Taking into account spin, the state of the system can be described by

$$|n, \ell, m, s, s_z\rangle$$

where $s$ and $s_z$ are, respectively, the total and $z$–component of the spin. Therefore, we get the first order energy correction

$$\Delta E = \langle 1, 0, 0, s', s'_z | \hat{H}_{\text{int}} | 1, 0, 0, s, s_z\rangle$$

$$= -\frac{8\pi}{3} \int d^3r \psi^*_{100}(\vec{r}) \delta(\vec{r}) \psi_{100}(\vec{r}) \langle s', s'_z | \vec{\mu}_e \cdot \vec{\mu}_p | s, s_z\rangle$$

$$= -\frac{8\pi}{3} \left( \frac{ge}{2mc} \right)^2 |\psi_{100}(0)|^2 \langle s', s'_z | \hat{S}_e \cdot \hat{S}_p | s, s_z\rangle$$

Now,

$$\hat{S}_e \cdot \hat{S}_p = \frac{1}{2} (S^2 - S^2_e - S^2_p) = \frac{\hbar^2}{2} (S(S + 1) - 3/2)$$

and therefore is diagonal in this basis. We then have

$$\Delta E = -\frac{8\pi}{3} \left( \frac{ge}{2mc} \right)^2 \left( \frac{1}{2a_0} \right)^3 \frac{\hbar^2}{2} (S(S + 1) - 3/2)$$

Now, positronium has a singlet state, $S = 0$, $S_z = 0$ and a triplet state $S = 1$, $S_z = 0$, ±1.
For the singlet state
\[ \Delta E_0 = 2\pi \left( \frac{e}{mc} \right)^2 \left( \frac{1}{2a_0} \right)^3 \hbar^2 = \frac{1}{4} \left( \frac{e^2}{hc} \right)^2 \frac{e^2}{a_0} = \frac{1}{4} mc^2 \alpha^4 > 0 \]

For the triplet state
\[ \Delta E_1 = -\frac{1}{12} \left( \frac{e^2}{hc} \right)^2 \frac{e^2}{a_0} = -\frac{1}{12} mc^2 \alpha^4 < 0 \]

Thus, the triplet ground state has the lowest energy and the energy splitting of the perturbed ground state levels is
\[ \Delta E_0 - \Delta E_1 = \Delta E = \frac{1}{3} mc^2 \alpha^4 = \frac{1}{3} (0.51 \times 10^6 \text{eV}) \left( \frac{1}{137} \right)^4 = 4.83 \times 10^{-4} \text{eV} \]

corresponding to
\[ \frac{\Delta E}{\hbar} = \nu = 1.17 \times 10^{11} \text{Hz} = 117 \text{GHz} \]

### 10.9.40 Two coupled spins

Two oppositely charged spin−1/2 particles (spins \( \vec{s}_1 = h\vec{\sigma}_1/2 \) and \( \vec{s}_2 = h\vec{\sigma}_2/2 \)) are coupled in a system with a spin-spin interaction energy \( \Delta E \). 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
\[ |1\rangle = |+\rangle_1 |+\rangle_2 , \quad |2\rangle = |+\rangle_1 |-\rangle_2 , \quad |3\rangle = |-\rangle_1 |+\rangle_2 , \quad |4\rangle = |-\rangle_1 |-\rangle_2 \]

where
\[ \sigma_{ix} |\pm\rangle_i = \mp |\pm\rangle_i , \quad \sigma_{ix} |\mp\rangle_i = \pm |\mp\rangle_i \]
and
\[ \sigma_{ix}\sigma_{2x}|1\rangle = \sigma_{ix}\sigma_{2x}|+\rangle_1 |+\rangle_2 = (\sigma_{ix}\sigma_{2x}|+\rangle_1)(\sigma_{2x}\sigma_{ix}|+\rangle_2) = |-\rangle_1 |-\rangle_2 = |4\rangle \]

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 \( \vec{\sigma}_i = 2\vec{s}_i/\hbar \) are
\[ |1'\rangle = |+\rangle_1 |+\rangle_2 = |1\rangle , \quad |2'\rangle = d |+\rangle_1 |-\rangle_2 + c |+\rangle_1 |-\rangle_2 = d |3\rangle + c |2\rangle \]
\[ |3'\rangle = c |-\rangle_1 |+\rangle_2 - d c |-\rangle_1 |+\rangle_2 = c |3\rangle - d |2\rangle , \quad |4'\rangle = |-\rangle_1 |-\rangle_2 = |4\rangle \]

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where
\[ \vec{\sigma}_i |\pm\rangle_i = |\pm\rangle_i \]
as stated above and
\[ d = \frac{1}{\sqrt{2}} \left( 1 - \frac{x}{\sqrt{1 + x^2}} \right)^{1/2}, \quad c = \frac{1}{\sqrt{2}} \left( 1 + \frac{x}{\sqrt{1 + x^2}} \right)^{1/2}, \quad x = \frac{\mu_0 B(g_2 - g_1)}{\Delta E} \]

(b) Find the energy eigenvalues associated with the 4 states.

We have
\[ \vec{\mu} = g_i \mu_0 \vec{S}_i, \quad \vec{S}_i = \frac{\hbar}{2} \vec{\sigma}_i, \quad \vec{B} = B \vec{\hat{z}} \]
\[ \hat{H} = \frac{\Delta E}{4} \vec{\sigma}_1 \cdot \vec{\sigma}_2 - (\vec{\mu}_1 + \vec{\mu}_2) \cdot \vec{B} \]
\[ = \frac{\Delta E}{4} (\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}) - \frac{1}{2} \mu_0 B (g_1 \sigma_{1z} + g_2 \sigma_{2z}) \]

In the \( \vec{\sigma}_z \) basis, we have 1-particle states with these properties
\[ \vec{\sigma}_x |+\rangle = |+\rangle, \quad \vec{\sigma}_x |\rangle = |\pm\rangle \]
\[ \vec{\sigma}_y |+\rangle = i|\pm\rangle, \quad \vec{\sigma}_y |\rangle = -i|\pm\rangle \]
\[ \vec{\sigma}_z |+\rangle = |+\rangle, \quad \vec{\sigma}_z |\rangle = |\pm\rangle \]

We now define the 2-particle basis
\[ |1\rangle = |+\rangle_1 |+\rangle_2, \quad |2\rangle = |+\rangle_1 |\rangle_2, \quad |3\rangle = |\rangle_1 |+\rangle_2, \quad |4\rangle = |\pm\rangle_1 |\pm\rangle_2 \]

We then have
\[ \hat{\sigma}_{1z} \hat{\sigma}_{2z} |1\rangle = \hat{\sigma}_{1z} \hat{\sigma}_{2z} |+\rangle_1 |+\rangle_2 = |+\rangle_1 |+\rangle_2 = |+\rangle_1 |+\rangle_2 \]
\[ \hat{\sigma}_{1z} \hat{\sigma}_{2z} |2\rangle = |+\rangle_1 |\rangle_2 = |+\rangle_1 |\rangle_2 \]
\[ \hat{\sigma}_{1z} \hat{\sigma}_{2z} |3\rangle = |\rangle_1 |+\rangle_2 = |\rangle_1 |+\rangle_2 \]
\[ \hat{\sigma}_{1z} \hat{\sigma}_{2z} |4\rangle = |\pm\rangle_1 |\pm\rangle_2 \]

Then
\[ \hat{\hat{H}} |1\rangle = (\frac{\Delta E}{4} - \frac{\mu_0 B(g_1 + g_2)}{2}) |1\rangle \]
\[ \hat{H}_{11} = \frac{\Delta E}{4} - \frac{\mu_0 B(g_1 + g_2)}{2}, \quad H_{12} = H_{21} = H_{31} = H_{31} = H_{41} = 0 \]
\[ \hat{H} |2\rangle = (\frac{\Delta E}{4} - \frac{\mu_0 B(g_1 - g_2)}{2}) |2\rangle + \frac{\Delta E}{2} |3\rangle \]
\[ \hat{H}_{22} = \frac{\Delta E}{4} - \frac{\mu_0 B(g_1 - g_2)}{2}, \quad H_{12} = H_{21} = H_{24} = H_{42} = 0, \quad H_{23} = H_{32} = \frac{\Delta E}{2} \]
\[ \hat{H} |3\rangle = (\frac{\Delta E}{4} + \frac{\mu_0 B(g_1 - g_2)}{2}) |3\rangle + \frac{\Delta E}{2} |2\rangle \]
\[ \hat{H}_{33} = \frac{\Delta E}{4} + \frac{\mu_0 B(g_1 - g_2)}{2}, \quad H_{31} = H_{31} = H_{34} = H_{43} = 0, \quad H_{23} = H_{32} = \frac{\Delta E}{2} \]
\[ \hat{H} |4\rangle = (\frac{\Delta E}{4} + \frac{\mu_0 B(g_1 + g_2)}{2}) |4\rangle \]
\[ \hat{H}_{44} = \frac{\Delta E}{4} + \frac{\mu_0 B(g_1 + g_2)}{2}, \quad H_{41} = H_{42} = H_{42} = H_{34} = H_{43} = 0 \]

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We then have the $\hat{H}$ matrix in the 2-particle basis

$$H = \begin{pmatrix} \frac{\Delta E}{4} - \frac{\mu_0 E}{2} (g_1 + g_2) & 0 & -\frac{\Delta E}{4} + \frac{\mu_0 E}{2} (g_1 - g_2) \\ 0 & \frac{\Delta E}{4} - \frac{\mu_0 E}{2} (g_1 - g_2) & 0 \\ -\frac{\Delta E}{4} - \frac{\mu_0 E}{2} (g_1 - g_2) & 0 & -\frac{\Delta E}{4} + \frac{\mu_0 E}{2} (g_1 - g_2) \\ \frac{\Delta E}{4} + \frac{\mu_0 E}{2} (g_1 + g_2) & 0 & 0 \end{pmatrix}$$

**Eigenvalues:** We already have two diagonal elements so that

$$E_1 = \frac{\Delta E}{4} - \frac{1}{2} \mu_0 B (g_1 + g_2), \quad E_4 = \frac{\Delta E}{4} + \frac{1}{2} \mu_0 B (g_1 + g_2)$$

We obtain the characteristic equation for the other two eigenvalues from the $2 \times 2$ matrix. We have

$$\left( -\frac{\Delta E}{4} - \frac{1}{2} \mu_0 B (g_1 - g_2) - E \right) \left( -\frac{\Delta E}{4} + \frac{1}{2} \mu_0 B (g_1 - g_2) - E \right) - \left( \frac{\Delta E}{2} \right)^2 = 0$$

$$E^2 + \frac{\Delta E}{2} E + \left( \frac{\Delta E}{4} \right)^2 - \frac{1}{4} (\mu_0 B (g_1 - g_2))^2 - \left( \frac{\Delta E}{2} \right)^2 = 0$$

$$E_{\pm} = -\frac{\Delta E}{4} \pm \frac{1}{2} \sqrt{\left( \frac{\Delta E}{2} \right)^2 + (\mu_0 B (g_1 - g_2))^2 + \frac{3}{4} (\Delta E)^2}$$

where

$$x = \frac{\mu_0 B (g_1 - g_2)}{\Delta E}$$

**Eigenvectors:** We then have the following complete solution

$$|\bar{1}\rangle = |1\rangle \rightarrow E_1 = \frac{\Delta E}{4} - \frac{1}{2} \mu_0 B (g_1 + g_2)$$

$$|\bar{2}\rangle = d |3\rangle + c |2\rangle \rightarrow E_2 = -\frac{\Delta E}{4} \left( 1 - 2 \sqrt{1 + x^2} \right)$$

$$|\bar{3}\rangle = d |3\rangle - c |2\rangle \rightarrow E_3 = -\frac{\Delta E}{4} \left( 1 + 2 \sqrt{1 + x^2} \right)$$

$$|\bar{4}\rangle = |4\rangle \rightarrow E_4 = \frac{\Delta E}{4} + \frac{1}{2} \mu_0 B (g_1 + g_2)$$

where

$$c^2 + d^2 = 1 \quad \langle 2 | 3 \rangle = 0 \quad \text{(orthogonal)}$$

Now we can determine $c$ and $d$ as follows.

$$\hat{H} |2\rangle = E_2 |2\rangle$$

$$\hat{H} (d |3\rangle + c |2\rangle) = -\frac{\Delta E}{4} \left( 1 - 2 \sqrt{1 + x^2} \right) (d |3\rangle + c |2\rangle)$$

$$d \left( -\frac{\Delta E}{4} + \frac{1}{2} \mu_0 B (g_1 - g_2) \right) |3\rangle + \frac{\Delta E}{2} |2\rangle = c \left( -\frac{\Delta E}{4} - \frac{1}{2} \mu_0 B (g_1 - g_2) \right) |2\rangle + \frac{\Delta E}{2} |3\rangle$$

$$= -\frac{\Delta E}{4} \left( 1 - 2 \sqrt{1 + x^2} \right) (d |3\rangle + c |2\rangle)$$

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→ d − \left( \frac{1}{2} + x \right) c = -\frac{1}{2} \left( 1 - 2\sqrt{1 + x^2} \right) c

→ c − \left( \frac{1}{2} - x \right) d = \frac{1}{2} \left( 1 - 2\sqrt{1 + x^2} \right) d

We then find

\begin{align*}
c &= \frac{1}{\sqrt{2}} \left( 1 + \frac{x}{\sqrt{1 + x^2}} \right)^{1/2}, \\
d &= \frac{1}{\sqrt{2}} \left( 1 - \frac{x}{\sqrt{1 + x^2}} \right)^{1/2}
\end{align*}

(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.

For \( \mu_0 B/\Delta E << 1 \) or \( x \ll 1 \) we have

\begin{align*}
E_1 &= \frac{\Delta E}{4} - \frac{1}{2} \mu_0 B(g_1 + g_2) \\
E_2 &= -\frac{\Delta E}{4} (1 - 2\sqrt{1 + x^2}) = -\frac{\Delta E}{4} (-1 - x^2) = -\frac{\Delta E}{4} \left( -1 - \left( \frac{\mu_0 B(g_1 - g_2)}{\Delta E} \right)^2 \right) \\
E_3 &= -\frac{\Delta E}{4} (1 + 2\sqrt{1 + x^2}) = -\frac{\Delta E}{4} (2 + x^2) = -\frac{\Delta E}{4} \left( 2 + \left( \frac{\mu_0 B(g_1 - g_2)}{\Delta E} \right)^2 \right) \\
E_4 &= \frac{\Delta E}{4} + \frac{1}{2} \mu_0 B(g_1 + g_2)
\end{align*}

so that in the limit \( x \to 0 \) we have

\begin{align*}
E_1 &= \frac{\Delta E}{4} = E_2 = E_4 \\
E_3 &= -\frac{3\Delta E}{4}
\end{align*}

or two distinct levels (one is 3-fold degenerate).

For \( \mu_0 B/\Delta E >> 1 \) or \( x \gg 1 \) we have

\begin{align*}
E_1 &= \frac{\Delta E}{4} - \frac{1}{2} \mu_0 B(g_1 + g_2) = -\frac{1}{2} \mu_0 B(g_1 + g_2) \\
E_2 &= -\frac{\Delta E}{4} (1 - 2\sqrt{1 + x^2}) = -\frac{\Delta E}{4} (-2x) = -\frac{\Delta E}{4} \left( \frac{\mu_0 B(g_1 - g_2)}{\Delta E} \right)^2 \\
E_3 &= -\frac{\Delta E}{4} (1 + 2\sqrt{1 + x^2}) = -\frac{\Delta E}{4} (2x) = -\frac{\Delta E}{4} \left( \frac{\mu_0 B(g_1 - g_2)}{\Delta E} \right)^2 \\
E_4 &= \frac{\Delta E}{4} + \frac{1}{2} \mu_0 B(g_1 + g_2) = \frac{1}{2} \mu_0 B(g_1 + g_2)
\end{align*}

or 4 distinct, non-degenerate levels. An illustrative plot is obtained by choosing some convenient numbers

\[ \Delta E = 1.0 \quad , \quad g_1 = 2.0 \quad , \quad g_2 = 1.0 \quad , \quad \mu_0 = 1.0 \]

so that

\begin{align*}
E_1 &= \frac{1}{4} - \frac{3}{2} B \\
E_2 &= -\frac{1}{4} \left( 1 - 2\sqrt{1 + B^2} \right) \\
E_3 &= -\frac{1}{4} \left( 1 + 2\sqrt{1 + B^2} \right) \\
E_4 &= \frac{1}{4} + \frac{3}{2} B
\end{align*}

as shown below.
10.9.41 Perturbed Linear Potential

A particle moving in one-dimension is bound by the potential

\[ V(x) = \begin{cases} \alpha x & x > 0 \\ \infty & x < 0 \end{cases} \]

where \( \alpha > 0 \) 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.

We have

\[ H = \frac{p^2}{2m} + V \]

where

\[ V(x) = \begin{cases} \alpha x & x > 0 \\ \infty & x < 0 \end{cases} \]
We now write
\[ V = V_0 + V_1 \]
where
\[ V_0(x) = \begin{cases} \frac{b}{x^2} & x > 0 \\ \infty & x < 0 \end{cases} \]
\[ V_1(x) = \begin{cases} ax - bx^2 & x > 0 \\ \infty & x < 0 \end{cases} \]
We then assume that the unperturbed system
\[ H_0 = \frac{p^2}{2m} + V_0 \]
These unperturbed solutions must have \( \psi(0) = 0 \) due to the infinite wall. The solutions are the the standard harmonic oscillator solution which vanish at the origin, i.e., all the odd solutions. Thus, the unperturbed system has states \( |n\rangle \), \( n = 1, 3, 5, \ldots \) with corresponding energies \( E_n^{(0)} = \hbar \omega (n + 1/2) \), \( n = 1, 3, 5, \ldots \).

The perturbation is \( V_1(x) \). For \( x > 0 \) we can write
\[ V_1 = ax - bx^2 = ax_0(a + a^+ - bx_0^2(a + a^+)^2 \]
Remembering that the solutions are only valid for \( x > 0 \), which introduces a factor of 2, we have the first order energy corrections
\[ E_n^{(1)} = \frac{\langle n| V_1 |n\rangle}{2} \]
\[ = -b\hbar x_0^2 \langle n| (a + a^+ a^+) |n\rangle /2 = -b\hbar x_0^2 \langle n| (2a^+ a + 1) |n\rangle /2 \]
\[ = -b\hbar x_0^2 (n + 1/2) \quad n = 1, 3, 5, \ldots \]

10.9.42 The ac-Stark Effect

Suppose an atom is perturbed by a monochromatic electric filed oscillating at frequency \( \omega_L \), \( \vec{E}(t) = E_z \cos \omega_L t \hat{e}_z \) (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).
(i) **The classical picture.** Consider first the *Lorentz oscillator* model of the atom - a charge on a spring - with natural resonance at $\omega_0$. The Hamiltonian for the system is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2z^2 - d \cdot \vec{E}(t)$$

where $d = -ez$ is the dipole.

(a) Ignoring damping of the oscillator, use Newton’s Law to show that the induced dipole moment is

$$\vec{d}_{\text{induced}}(t) = \alpha \vec{E}(t) = \alpha E_z \cos \omega_L t$$

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*.

The incident field will drive oscillations of the charge at frequency $\omega_L$. The equation of motion is

$$\ddot{z} + \omega_0^2z = -\frac{e}{m}E_z \cos \omega_L t$$

We shift to complex amplitudes via

$$z \equiv \Re(Z_0 e^{-i\omega_L t})$$

This gives

$$(-\omega_L^2 + \omega_0^2)Z_0 = -\frac{e}{m}E_z \rightarrow Z_0 = -\frac{e}{m\omega_0^2 - \omega_L^2}E_z$$

The induced dipole moment oscillating at drive-frequency $\omega_L$ is

$$d_{\text{induced}}(t) = \Re(-eZ_0 e^{-i\omega_L t}) = \frac{e^2}{m\omega_0^2 - \omega_L^2}E_z \cos \omega_L t$$
or

\[ d_{induced}(t) = \alpha \vec{E}(t) \rightarrow \alpha = \frac{e^2}{m} \frac{1}{\omega_0^2 - \omega_L^2} = (2\omega_0 + \Delta)(-\Delta) \approx -2\omega_0 \Delta \]

In the near resonance approximation, we let \( \Delta = \omega_L - \omega_0 \)

which is the detuning factor and we have

\[ \Delta \ll \omega_0 \sim |\omega_L| \]

This implies that

\[ \omega_0^2 - \omega_L^2 = (\omega_0 + \omega_L)(\omega_0 - \omega_L) = (2\omega_0 + \Delta)(-\Delta) \approx -2\omega_0 \Delta \]

to first order in \( \Delta \ll \omega_0 \). Therefore we have

\[ \alpha \approx -\frac{e^2}{2m\omega_0\Delta} \]

(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

\[ \bar{H} = -\frac{1}{4} \alpha E^2 \]

Note the factor of 1/2 arises because energy is required to create the dipole.

The total energy is

\[ H = \frac{1}{2} m \dot{z}^2 + \frac{1}{2} m \omega_0^2 z^2 - \vec{d} \cdot \vec{E} \]

or

\[ H = \frac{1}{2} m(\omega_0^2 - \omega_L^2) z^2 - \vec{d} \cdot \vec{E} \]

\[ = \frac{1}{2} m(\omega_0^2 - \omega_L^2) \frac{e^2}{m^2 \omega_0^2 - \omega_L^2} \frac{1}{2} E^2 - \alpha E^2 \]

\[ = \frac{1}{2} \alpha E^2 - \alpha E^2 = -\frac{1}{2} \alpha E^2 \]

Therefore,

\[ H = -\frac{1}{2} \alpha E^2(t) = -\frac{1}{2} d_{ind}(t) \cdot \vec{E}(t) \]
Time averaging using
\[ \cos^2 \omega_L t = \frac{1}{2} \]
we get
\[ \hat{H} = -\frac{1}{4} \alpha E_z^2 \]

(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 \( \hat{H}_{atom} = -\hbar \Delta |e\rangle \langle e| \) is the *unperturbed* atomic Hamiltonian and \( \hat{H}_{int} = -\frac{\hbar \Omega}{2} (|e\rangle \langle g| + |g\rangle \langle e|) \) is the dipole-interaction with \( \hbar \Omega = \langle e| \vec{d} |g\rangle \cdot \vec{E} \).

(a) Find the *exact* energy eigenvalues and eigenvectors for this simple two dimensional Hilbert space and plot the levels as a function of \( \Delta \). These are known as the atomic *dressed states*.

Given a two level atom with \( \Delta \ll \omega_0 \) and thus \( \Delta \ll |\omega_L| \) as shown below

(we ignore all other levels in this system), then the effective Hamiltonian is \( \hat{H} = \hat{H}_0 + \hat{H}_1 \) where
\[ \hat{H}_0 = \hat{H}_{atom} = -\hbar \Delta |e\rangle \langle e| \rightarrow \text{the "unperturbed atom"} \]
\[ \hat{H}_1 = -\frac{\hbar \Omega}{2} (|e\rangle \langle g| + |g\rangle \langle e|) \rightarrow \text{the "laser interaction"} \]
with
\[ \Omega = \frac{\langle e| \vec{d} |g\rangle \cdot \vec{E}}{\hbar} \rightarrow \text{the "Rabi frequency"} \]

This simple 2-dimensional problem can be solved exactly. We can write the matrix representation in the \( \{|e\rangle, |g\rangle\} \) basis as
\[ H = -\hbar \begin{pmatrix} \Delta & \Omega/2 \\ \Omega/2 & 0 \end{pmatrix} = -\hbar \begin{pmatrix} \Delta/2 & \Delta/2 \hat{\sigma}_z + \Omega/2 \hat{\sigma}_x \\ \Delta/2 \hat{\sigma}_z + \Omega/2 \hat{\sigma}_x & 0 \end{pmatrix} \]
\[ = -\hbar \frac{\Delta}{2} \hat{I} - \hbar \frac{\Omega}{2} \hat{\sigma} \cdot \vec{\sigma} \]
where
\[ \vec{\Omega} = \Delta \hat{e}_z + \Omega \hat{e}_x \]
is the generalized Rabi frequency and
\[ \hat{\Omega} \equiv |\vec{\Omega}| = \sqrt{\Omega^2 + \Delta^2} \]
so that
\[ \frac{\vec{\Omega}}{\hat{\Omega}} \equiv \cos \theta \hat{e}_z + \sin \theta \hat{e}_x \]
with
\[ \tan \theta = \frac{\Omega}{\Delta} \]
We then have the eigenvalues
\[ E_{\pm} = -\frac{\hbar}{2} (\Delta \pm \hat{\Omega}) = -\frac{\hbar}{2} (\Delta \pm \sqrt{\Omega^2 + \Delta^2}) \]
and the eigenvectors
\[ |\pm\rangle = \cos \frac{\theta}{2} |e\rangle + \sin \frac{\theta}{2} |g\rangle \]
A plot looks like:

This is typical anti-crossing behavior (we have seen this earlier). At \( \Delta = 0 \), \(|e\rangle\) and \(|g\rangle\) are degenerate in the absence of coupling. The field breaks the degeneracy into symmetric and antisymmetric superpositions.

Note that for \( \Delta < 0 \) (called "red detuning") \(|e\rangle\) is shifted up and \(|g\rangle\) down (called level repulsion).

For \( \Delta > 0 \) (called "blue detuning") the reverse occurs and implies
level attraction.

We note that in static perturbation theory the levels always repel due to the perturbation. The above calculation agrees with this since in the D.C. limit, $\Delta$ is negative.

(b) Expand your solution in (a) to lowest nonvanishing order in $\Omega$ to find the perturbation to the energy levels. Under what conditions is this expansion valid?

We do an expansion in

$$\frac{\text{coupling matrix element}}{\text{energy level difference}} = \frac{\Omega}{\Delta} \ll 1$$

$$E_\pm = -\frac{\hbar}{2} \left( \Delta \pm \Delta \sqrt{1 + \frac{\Omega^2}{\Delta^2}} \right) \approx -\frac{\hbar}{2} \left( \Delta \pm \Delta \left( 1 + \frac{\Omega^2}{2\Delta^2} \right) \right)$$

so that

$$E_+ \approx -\hbar\Delta - \frac{\hbar\Omega^2}{4\Delta} , \quad E_- \approx \frac{\hbar\Omega^2}{4\Delta}$$

Thus, the lowest non-vanishing perturbation is second-order in $\Omega$.

(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 $\langle \vec{d} \rangle = a \vec{E}$ is given by

$$\alpha = -\frac{|\langle \vec{d} \rangle \vec{g} |^2}{\hbar\Delta}$$

so that the second order perturbation to the ground state is $E_g^{(2)} = -\alpha E_z^2$ as in part (b).

Using perturbation theory where

$$\hat{H}_1 = -\frac{\hbar\Omega}{2} (|e\rangle \langle g| + |g\rangle \langle e|)$$

we have

$0^{th}$-order:

$$E_e^{(0)} = -\hbar\Delta , \quad E_g^{(0)} = 0$$

$1^{st}$-order:

$$E_e^{(1)} = \langle e| \hat{H}_1 | e\rangle = 0 , \quad E_g^{(1)} = \langle g| \hat{H}_1 | g\rangle = 0$$

$2^{nd}$-order:

$$E_e^{(2)} = \frac{|\langle g| \hat{H}_1 | e\rangle |^2}{E_e^{(0)} - E_g^{(0)}} = \frac{\hbar^2 \Omega^2 / 4}{-\hbar\Delta} = -\frac{\hbar\Omega^2}{4\Delta}$$
\[ E_g^{(2)} = \frac{|\langle e| \hat{H}_1 |g \rangle|^2}{E_g^{(0)} - E_e^{(0)}} = \frac{\hbar^2 \Omega^2 / 4}{\hbar \Delta} = \frac{\hbar \Omega^2}{4 \Delta} \]

Thus, to second-order

\[ E_e = E_e^{(0)} + E_e^{(2)} = -\hbar \Delta - \frac{\hbar \Omega^2}{4 \Delta} \]

\[ E_g = E_g^{(0)} + E_g^{(2)} = \frac{\hbar \Omega^2}{4 \Delta} \]

as in (b).

**Mean Dipole:** We assume that the atom starts in the ground state. To first order

\[ \left\langle \tilde{\phi}_g \right\rangle = |g\rangle + |e\rangle \left\langle \frac{\langle e| \hat{H}_1 |g \rangle}{E_g^{(0)} - E_e^{(0)}} \right\rangle = \left| \phi_g^{(0)} \right\rangle + \left| \phi_g^{(1)} \right\rangle \]

Therefore

\[ \left| \tilde{\phi}_g \right\rangle = |g\rangle - \frac{\Omega}{2 \Delta} |e\rangle \quad \text{(unnormalized)} \]

Thus,

\[ \langle \tilde{d} \rangle = \frac{\left\langle \tilde{\phi}_g | \tilde{d} | \tilde{\phi}_g \right\rangle}{\left\langle \tilde{\phi}_g | \tilde{\phi}_g \right\rangle} = -\frac{\Omega^*}{2 \Delta} \frac{\langle e| \tilde{d} |g \rangle + \Omega \langle g| \tilde{d} |e \rangle}{1 + \frac{\Omega^2}{4 \Delta^2}} \]

Since

\[ \frac{\Omega^2}{4 \Delta^2} \ll 1 \]

we can write

\[ \langle \tilde{d} \rangle = -\frac{1}{2 \Delta} (\Omega^* \langle e| \tilde{d} |g \rangle + \Omega \langle g| \tilde{d} |e \rangle) \]

Then, to lowest order in

\[ \Omega = \frac{\langle e| \tilde{d} |g \rangle \cdot \vec{E}}{\hbar} \]

\[ \langle \tilde{d} \rangle = -\frac{|\langle e| \tilde{d} |g \rangle|^2}{\hbar \Delta} \vec{E} = \alpha \vec{E} \]

and

\[ E_g^{(2)} = \frac{\hbar \Omega^2}{4 \Delta} = \frac{|\langle e| \tilde{d} |g \rangle|^2}{4 \hbar \Delta} |\vec{E}|^2 = -\frac{1}{4} \alpha |\vec{E}|^2 \]

as in the classical calculation (b).
(d) Show that the ratio of the polarizability calculated classically in (b) and the quantum expression in (c) has the form

\[ f = \frac{\alpha_{\text{quantum}}}{\alpha_{\text{classical}}} = \frac{|\langle e | z | g \rangle|^2}{(\Delta z^2)_{\text{SHO}}} \]

where \((\Delta z^2)_{\text{SHO}}\) is the SHO zero point variance. This is also known as the oscillator strength.

We have

\[ f = \frac{\alpha_q}{\alpha_c} = \frac{|\langle e | \vec{d} | g \rangle|^2}{\hbar \Delta} \cdot \frac{2m\omega_0 \Delta e^2}{\hbar} = \frac{2m\omega_0}{\hbar} \cdot |\langle e | \vec{d} | g \rangle|^2 \]

Thus,

\[ f = \frac{|\langle e | \vec{d} | g \rangle|^2}{(\Delta z)^2_{\text{SHO}}} \]

where

\[ (\Delta z)_{\text{SHO}} = \frac{\hbar}{2m\omega_0} \]

For a multi-level atom with resonances \(\{\omega_i\}\)

\[ \alpha = \sum_i f(\omega_i)\alpha(\omega_i) \]

The oscillator strength satisfies the sum rule

\[ \sum_i f(\omega_i) = Z \quad (\text{atomic number}) \]

For hydrogen and the alkalies, the majority of the oscillator strength lies in the first \(s \rightarrow p\) transition. Thus, if the perturbation is far from any resonance, this transition will dominate.

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 monochromatic 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 \(\vec{E}(x, t) = \Re(\vec{E}(\vec{x})e^{-i\omega_L t})\), driving an atom near resonance on the transition \(|g; J_g \rangle \rightarrow |e; J_e \rangle\), 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:

$$
\hat{V}_{LS}(\vec{x}) = -\frac{1}{4} \vec{E}^*(\vec{x}) \cdot \hat{\alpha} \cdot \vec{E}(\vec{x})
$$

Here,

$$
\hat{\alpha} = -\frac{\hat{d}_{eg} \hat{d}_{eg}^*}{\hbar \Delta}
$$

is the atomic polarizability tensor operator, where $\hat{d}_{eg} = \hat{P}_e \hat{d} \hat{P}_g$ 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

$$
\hat{\alpha} = \hat{\alpha} \left( \sum_{q, M_g} |C_{M_g}^{M_g+q}|^2 \hat{ \epsilon }_q \ |g, J_g, M_g\rangle \langle g, J_g, M_g| \hat{ \epsilon }_q^* + \sum_{q \neq q', M_g} C_{M_g+q}^{M_g+q'} C_{M_g}^{M_g+q} \hat{ \epsilon }_{q'} \ |g, J_g, M_g + q - q'\rangle \langle g, J_g, M_g| \hat{ \epsilon }_{q'}^* \right)
$$

where

$$
\hat{\alpha} = -\frac{|\langle e; J_e \| d \| g; J_g \rangle|^2}{\hbar \Delta}
$$

and

$$
C_{M_g}^{M_e} = \langle J_e M_e \| q J_g M_g \rangle
$$

Explain physically, using dipole selection rules, the meaning of the expression for $\hat{\alpha}$.

Let us write the explicit representation in the basis of the magnetic sublevels:

$$
\hat{d}_{eg} = \hat{P}_e \hat{d} \hat{P}_g = \sum_{M_e = -J_e}^{J_e} \sum_{M_g = -J_g}^{J_g} \sum_{M_e} |e; J_e M_e\rangle \langle e; J_e M_e| \hat{d} \ |g; J_g M_g\rangle \langle g; J_g M_g|
$$

We can then make a spherical basis expansion

$$
\hat{d} = \sum_{q} (-1)^q \hat{ \epsilon }_{-q} d_q = \sum_{q} \hat{ \epsilon }_{q}^* d_q
$$

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which then implies that
\[
\hat{d}_{eg} = \sum_{M_e, M_g} \hat{e}_q^a \langle e; J_e M_e | \hat{d}_q | g; J_g M_g \rangle \langle e; J_e M_e \rangle \langle g; J_g M_g \rangle
\]

Aside: Wigner-Eckhart theorem:
\[
\langle e; J_e M_e | \hat{d}_q | g; J_g M_g \rangle = \langle e; J_e \| d \| g; J_g \rangle \langle J_e M_e | 1q J_g M_g \rangle
\]

Using the selection rule \( M_e = M_g + q \) we have
\[
\hat{d}_{eg} = \sum_{M_g, q} \hat{\epsilon}_q^{M_g+q} | e; J_e M_g + q \rangle \langle g; J_g M_g | \langle e \| d \| g \rangle
\]

where we have used a shorthand for the dipole CG coefficient
\[
\epsilon_{M_g+q}^{M_g} = \langle J_e M_g + q \big| 1q J_g M_g \rangle
\]

Similarly,
\[
\hat{d}_{ge} = \hat{\epsilon}_{-g}^q \sum_{M_g, q} \hat{\epsilon}_q^{M_g+q} | e; J_e M_g + q \rangle \langle g; J_g M_g | \langle e \| d \| g \rangle^*\]

which says that
\[
\hat{d}_{ge} \hat{d}_{eg} = \sum_{M_g, M_g', q, q'} \hat{\epsilon}_q^{M_g+q} \hat{\epsilon}_{-g}^{M_g'+q'} C_{M_g}^{M_g+q} C_{M_g'}^{M_g'+q'} | g; J_g M_g \rangle \langle e; J_e M_g' + q' \big| e; J_e M_g + q \rangle \langle g; J_g M_g | \langle e \| d \| g \rangle^2
\]

Now
\[
\langle e; J_e M_g' + q' | e; J_e M_g + q \rangle = \delta_{M_g'M_g, q' - q}
\]

This corresponds to the selection rule
\[
M_g' - M_g = q - q'
\]

which is just conservation of angular momentum \( \delta_{M_g', M_g - q - q'} \). Thus,
\[
\hat{d}_{ge} \hat{d}_{eg} = |\langle e \| d \| g \rangle|^2 \sum_{M_g} \sum_{q, q'} \hat{\epsilon}_q^{M_g+q} \hat{\epsilon}_{-g}^{M_g'+q'} C_{M_g}^{M_g+q} C_{M_g'}^{M_g'+q'} | g; J_g M_g + q - q' \rangle \langle g; J_g M_g | \langle e \| d \| g \rangle^2
\]

Putting this together, the polarizability tensor in a spherical basis representation is (explicitly writing the diagonal and off-diagonal terms):
\[
\hat{\alpha} = \hat{\alpha} + \sum_{q, M_g} \left( C_{M_g}^{M_g+q} \hat{\epsilon}_q^{M_g+q} \hat{\epsilon}_{-g}^{M_g+q} \langle g; J_g M_g \rangle \langle g, J_g, M_g \rangle \langle e; J_e M_e \rangle \langle e; J_e M_e | \hat{d}_q | g; J_g M_g \rangle \langle g; J_g M_g \rangle \hat{\epsilon}_q^{*} \right)
\]

where
\[
\hat{\alpha} = -\frac{|\langle e; J_e \| d \| g; J_g \rangle|^2}{\hbar \Delta}
\]

**Physical Picture:** We have this example (shown below)
Here the shift can be thought of as resulting from virtual absorption and emission of photons.

If the atom absorbs and reemits a photon of helicity $q$ this implies that it comes back to some state so that we have an oscillator strength $M_g \leftrightarrow M_e$.

If the atom absorbs a photon of helicity $q$ and emits $q'$, the deficit goes into atomic angular momentum.

**Example-diagonal term:**

Here the strength is

$$|C_{M_e=2, M_g=1}|^2$$

**Example-off diagonal term:**

Here the strength is

$$(C_0^1 C_1^1)$$

(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 $|g; J_g = 1 \rangle \rightarrow$
$|e; J_e = 2\rangle$ 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 $|g; J_g = 1/2\rangle \rightarrow |e; J_e = 3/2\rangle$ and comment.

In the plane-polarized case

$$\vec{E}(\vec{x}) = E_1 \vec{\epsilon}_L \cdot \hat{\alpha} \cdot \vec{\epsilon}_L$$

which implies that

$$\hat{V}_{LS} = -\frac{1}{4} |E_1|^2 \vec{\epsilon}_L \cdot \hat{\alpha} \cdot \vec{\epsilon}_L$$

**case (i):** we have linear polarization along $z$ : $\vec{\epsilon}_L = \vec{\epsilon}_z$. This implies that

$$\hat{V}_{LS} = -\frac{1}{4} |E_1|^2 \vec{\epsilon}_z \cdot \hat{\alpha} \cdot \vec{\epsilon}_z = -\frac{\tilde{\alpha}}{4} |E_1|^2 \sum_{M_g} |C_{M_g}^{M_e}|^2 |g; J_g M_g\rangle \langle g; J_g M_g|$$

Thus, we only have diagonal terms (as in the figure above)

**case (ii):** we have $|g; J_g = 1\rangle \rightarrow |e; J_e = 2\rangle$ as shown below:

```
-2  -1  0  1  2  \hspace{1cm} J_e = 2
\hline
-1  \sqrt{\frac{5}{2}}  \sqrt{\frac{1}{2}}  \sqrt{\frac{3}{2}}  \sqrt{\frac{1}{2}}  \hspace{1cm} J_g = 4
```

Here the relevant CG coefficients are $C_{M_g}^{M_e} = \langle 2M_g | 101M_g\rangle$ which implies for $\vec{\epsilon}_L = \vec{\epsilon}_z$, that $|J_g = 1\rangle \rightarrow |J_e = 2\rangle$.

The appropriate eigenvectors are the magnetic sublevels $|g; J_g\rangle$ and the corresponding eigenvalues are $V_1/2, 2V_1/3$. For $\Delta < 0$ which implies $V_1 < 0$ we have the shifted levels

```
M_g -1  0  1
```

**case:** $\vec{\epsilon}_L = \vec{\epsilon}_+ \text{ or } |J_g = 1\rangle \rightarrow |J_e = 2\rangle$ we have
The appropriate eigenvectors are $|J_g, M_g\rangle$ with eigenvalues $M_g = 1 : V_1/6$, $M_g = 0 : V_1/2$, $M_g = +1 : V_1$ with the shifted ($V_1 < 0$) level diagram below.

Case: $\vec{e}_L = \vec{e}_x$ or $|J_g = 1\rangle \rightarrow |J_g = 2\rangle$ we have

$$\vec{e}_x = \frac{-\vec{e}_+ + \vec{e}_-}{\sqrt{2}}$$

which is not one of the spherical basis and therefore we do not just have diagonal elements as shown below.

**Light-Shift Operator**: for $\vec{e}_L = \vec{e}_x = (-\vec{e}_+ + \vec{e}_-)/\sqrt{2}$

$$\hat{V}_L(\vec{x}) = V_1 \sum_{M_g, q} |C_{M_g}^{M_g+q}|^2 (\vec{e}_x \cdot \vec{e}_q) |M_g\rangle \langle M_g| (\vec{e}_q \cdot \vec{e}_x)$$

$$= V_1 \sum_{M_g, q} C_{M_g}^{M_g+q} C_{M_g}^{M_g+q} (\vec{e}_x \cdot \vec{e}_q) |M_g + q - q'\rangle \langle M_g| (\vec{e}_q' \cdot \vec{e}_x)$$

$$= \frac{V_1}{2} \left( \sum_{M_g} (|C_{M_g}^{M_g+1}|^2 + |C_{M_g}^{-M_g-1}|^2) |M_g\rangle \langle M_g| - \sum_{M_g} (|C_{M_g+2}^{-M_g+1}|^2 + |C_{M_g}^{-M_g+1}|^2) |M_g + 2\rangle \langle M_g+2| + H.C. \right)$$

$$= \frac{V_1}{2} \left( |0\rangle \langle 0| + \frac{1}{12} (7|1\rangle \langle 1| + 7|-1\rangle \langle -1| - |1\rangle \langle -1| - |-1\rangle \langle 1| \right)$$

Note we have simplified the notation $|M_g\rangle \equiv |J_g, M_g\rangle$.

The eigenvalues and eigenvectors in the basis $\{|0\rangle, |1\rangle, |-1\rangle\}$ are obtained...
as follows:

\[
\hat{V}_L = \frac{V_1}{2} \begin{pmatrix}
1 & \vdots & 0 & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \vdots & \frac{7}{12} & -\frac{1}{12} \\
0 & \vdots & -\frac{1}{12} & \frac{7}{12}
\end{pmatrix}
\]

Since this is block-diagonal, we need only diagonalize the $2 \times 2$ matrix. It has eigenvalues $\frac{1}{2}, \frac{2}{3})$. Therefore, the eigenvalues/eigenvectors for $\vec{\epsilon}_L = \vec{\epsilon}_x$, $|J_g = 1 \rangle \rightarrow |J_e = 2 \rangle$ are:

\[
\frac{V_1}{2} |0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
\]

\[
\frac{V_1}{2} \frac{|1\rangle + |\bar{1}\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}
\]

\[
\frac{2V_1}{3} \frac{|1\rangle - |\bar{1}\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}
\]

Thus, we see that the eigenvalues for $\vec{\epsilon}_L = \vec{\epsilon}_z$ and $\vec{\epsilon}_L = \vec{\epsilon}_x$ are equal, which is as it must be, since what direction we call $x$ or $y$ or $z$ is irrelevant, i.e., the choice of quantization axis is arbitrary.

What about the eigenvectors for the two cases? For $\vec{\epsilon}_L = \vec{\epsilon}_z$ with $z$–quantization, we found eigenvectors $|M_z = 0 \rangle, |M_z = \pm 1 \rangle$ with eigenvalues $2V_1/3$ and $V_1/2$ (doubly degenerate, respectively).

This means that for $\vec{\epsilon}_L = \vec{\epsilon}_x$ with $x$–quantization we must have eigenvectors $|M_x = 0 \rangle, |M_x = \pm 1 \rangle$ with eigenvalues $2V_1/3$ and $V_1/2$ (doubly degenerate, respectively).

Now $|M_z \rangle = \hat{D} |M_z \rangle$ where $\hat{D}$ is a rotation matrix (operator).

For $J_g = 1$ we can explicitly calculate the rotation matrix, or use symmetry arguments via the spherical basis,

\[
|1, M_x = 0 \rangle = -\frac{i}{\sqrt{2}} (|1, M_z = +1 \rangle - |1, M_z = -1 \rangle)
\]

\[
|1, M_x = \pm 1 \rangle = -\frac{i}{\sqrt{2}} \left( \pm |1, M_z = 0 \rangle + \frac{1}{\sqrt{2}} |1, M_z = +1 \rangle + |1, M_z = -1 \rangle \right)
\]

Thus,

\[
\hat{V}_L |1, M_x = 0 \rangle = \frac{2}{3} V_1 |1, M_x = 0 \rangle
\]

\[
\hat{V}_L |1, M_x = \pm 1 \rangle = \frac{1}{2} V_1 |1, M_x = \pm 1 \rangle
\]

so it all makes sense.
Let us repeat this for the case: $|g; J_g = 1/2 \rightarrow |e; J_e = 3/2$ as shown below (with CG coefficients for dipole transitions):

**case (i):** $\vec{e}_L = \vec{e}_z$. We have eigenvectors $|J_g, M_g = \pm 1/2\rangle$ with eigenvalues $2V_1/3$ (doubly degenerate).

**case (ii):** $\vec{e}_L = \vec{e}_+$. We have eigenvectors $|J_g, M_g = \pm 1/2\rangle$ with eigenvalues $|J_g, M_g = +1/2\rangle V_1$ and $|J_g, M_g = -1/2\rangle V_1/3$.

**case (ii):** $\vec{e}_L = (-\vec{e}_+ + \vec{e}_-)/\sqrt{2}$. Unlike the $J_g h = 1$ case, the light-shift operator is diagonal here, since there are no $\Delta M_g = \pm 2$ matrix elements possible in the ground state, i.e.,

$$
\hat{V}_{LS} = \frac{V_1}{2} \sum_{M_g} (|C_{M_g}^{M_g+1}|^2 + |C_{M_g}^{M_g-1}|^2) |J_g M_g \rangle \langle J_g M_g |
$$

$$
= \frac{V_1}{2} ((1 + 1/3) |1/2\rangle \langle 1/2| + (1/3 + 1) |−1/2\rangle \langle −1/2|)
$$

$$
= \frac{2V_1}{3} (|1/2\rangle \langle 1/2| + |−1/2\rangle \langle −1/2|)
$$

This implies eigenvectors $|J_g, M_g = \pm 1/2\rangle$ with eigenvalues $|J_g, M_g = \pm 1/2\rangle$ with eigenvalues $2V_1/3$ (doubly degenerate). This is the same as the case $\vec{e}_L = \vec{e}_z$ as it must be.

(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, vector, and rank-2 irreducible tensor interactions,

$$
\hat{V}_{LS} = \frac{1}{4} \left( |\vec{E}(\vec{x})|^2 \hat{\alpha}^{(0)} + (\vec{E}^*(\vec{x}) \times \vec{E}(\vec{x}) \cdot \hat{\alpha}^{(1)} + \vec{E}^*(\vec{x}) \cdot \hat{\alpha}^{(2)} \cdot \vec{E}(\vec{x}) \right)
$$

where

$$
\hat{\alpha}^{(0)} = \frac{\hat{\vec{d}}_{ge} \cdot \hat{\vec{d}}_{eg}}{-3h\Delta}, \quad \hat{\alpha}^{(1)} = \frac{\hat{\vec{d}}_{ge} \times \hat{\vec{d}}_{eg}}{-2h\Delta}
$$

and

$$
\hat{\alpha}^{(2)}_{ij} = \frac{1}{-h\Delta} \left( \frac{\hat{\vec{d}}_{ge}^i \hat{\vec{d}}_{eg}^j + \hat{\vec{d}}_{ge}^j \hat{\vec{d}}_{eg}^i}{2} - \hat{\alpha}^{(0)} \delta_{ij} \right)
$$

The polarizability tensor can be written in terms of irreducible tensors. Let

$$
\hat{T}_{ij} = \hat{d}_{ge}^i \hat{d}_{eg}^j
$$
which is the outer product of two vectors. Now any such Cartesian tensors can be expanded in terms of irreducible tensors, i.e.,
\[ \hat{T}_{ij} = \hat{T}^{(0)}_{ij} + \hat{T}^{(1)}_{ij} + \hat{T}^{(2)}_{ij} \]
where
\[ \hat{T}^{(0)}_{ij} = \text{Trace}(\hat{T}_{ij}) \frac{\delta_{ij}}{3} = \frac{1}{3} \hat{\vec{d}}_i \cdot \hat{\vec{d}}_j \]
\[ \hat{T}^{(1)}_{ij} = \frac{\hat{d}^i_{ge} \hat{d}^j_{eg} - \hat{d}^i_{eg} \hat{d}^j_{ge}}{2} = \frac{1}{2} \epsilon_{ijk} (\hat{\vec{d}}_i \times \hat{\vec{d}}_j)_k \text{ antisymmetric} \]
\[ \hat{T}^{(2)}_{ij} = \frac{\hat{d}^i_{ge} \hat{d}^j_{eg} + \hat{d}^i_{eg} \hat{d}^j_{ge}}{2} = \frac{1}{2} \epsilon_{ijk} (\hat{\vec{d}}_i \times \hat{\vec{d}}_j)_k - \frac{1}{3} \hat{\vec{d}}_i \cdot \hat{\vec{d}}_j \text{ symmetric and traceless} \]
Thus, with
\[ \hat{\alpha}_{ij} = -\frac{1}{\hbar \Delta} \hat{T}_{ij} \]
we arrive at the desired expansion
\[ \hat{V}_{LS} = -\frac{1}{4} \hat{E}^* \cdot \hat{\alpha} \cdot \hat{E} = -\frac{1}{4} \hat{E}^* E_j \hat{\alpha}_{ij} \]
\[ = -\frac{1}{4} (\hat{\alpha}^{(0)} |\hat{E}(\vec{x})|^2 + \hat{\alpha}^{(1)} \cdot (\hat{E}^* \times \hat{E}) + \hat{E}^* (\vec{x}) \cdot \hat{\alpha}^{(2)} \cdot \hat{E}(\vec{x}) \]
where
\[ \hat{\alpha}^{(k)} = -\frac{1}{\hbar \Delta} \hat{T}^{(k)}_{ij} \]

(d) For the particular case of \( |g; J_g = 1/2 \rangle \rightarrow |e; J_e = 3/2 \rangle \), 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,
\[ \hat{V}_{LS} = V_0(\vec{x}) \hat{I} + \vec{B}_{fict}(\vec{x}) \cdot \vec{\sigma} \]
where
\[ V_0(\vec{x}) = \frac{2}{3} U_1 |\vec{\varepsilon}_L(\vec{x})|^2 \rightarrow \text{proportional to field intensity} \]
and
\[ \vec{B}_{fict}(\vec{x}) = \frac{1}{3} U_1 \left( \vec{\varepsilon}_L^*(\vec{x}) \times \vec{\varepsilon}_L(\vec{x}) \right) \rightarrow \text{proportional to field ellipticity} \]
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 \( |g; J_g = 1/2 \rangle \rightarrow |e; J_e = 3/2 \rangle \).
For the particular case \( |g; J_g = 1/2 \rangle \to |e; J_e = 3/2 \rangle \), \( \hat{V}_{LS} \) acts on the ground state manifold \{\( |J_g = 1/2 \rangle, |J_g = -1/2 \rangle \}\). The rank-2 part
\[
\hat{V}^{(2)}_{LS} = -\frac{1}{4} E^*_i E_j \hat{\alpha}^{(2)}_{ij}
\]
has matrix elements
\[
\langle J_g = 1/2, M'_g | \hat{V}^{(2)}_{LS} | J_g = 1/2, M_g \rangle = \langle 1/2 \| \hat{V}^{(2)}_{LS} \| 1/2 \rangle \langle 1/2 M'_g \| 2q1/2 M_g \rangle
\]
where the CG coefficient \( \langle 1/2 M'_g \| 2q1/2 M_g \rangle \) vanishes by the triangle inequality. Thus,
\[
-\frac{1}{4} (\hat{\alpha}^{(0)} |E(\vec{x})|^2 + \hat{\alpha}^{(1)} \cdot (\vec{E}^* \times \vec{E})
\]
where the first term is a scalar and the second term is a vector.

Acting on spin\(-1/2\), the scalar part must be proportional to the identity and the vector part to \( \hat{\vec{\sigma}} \) since any operator acting on the 2-dimensional Hilbert space is of this form. Thus,
\[
\hat{V}_{LS} = V_0(\vec{x}) \hat{I} + \vec{B}_{eff}(\vec{x}) \cdot \hat{\vec{\sigma}}
\]
where
\[
V_0(\vec{x}) = \frac{1}{2} Tr(\hat{V}_{LS}) , \quad \vec{B}_{eff}(\vec{x}) = \frac{1}{2} Tr(\hat{V}_{LS}) \hat{\vec{\sigma}}
\]

### 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 \( \lambda \) is a variational parameter. to estimate the ground state energy. Compare the result with the exact answer.

The wave function \( \psi(x) = |a|^\lambda - |x|^\lambda \) is symmetric, and it is thus sufficient to integrate over the interval \([0, a]\). The energy is
\[
E = -\frac{\hbar^2}{2m} \int_0^a dx \psi'' \int_0^a dx |\psi|^2 = -\frac{\hbar^2}{2m} \frac{A}{B}
\]
where \( \prime = d/dx \). We calculate \( A \) and \( B \) using \( \psi' = -\lambda x^{\lambda-1} \):
\[
A = \int_0^a dx \psi'' = \int (\psi \psi')' - \int (\psi')^2 = 0 - \frac{\chi^2 a^{2\lambda-1}}{2\lambda - 1}
\]

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\[ B = \int_0^a dx \psi^2 = \int_0^a dx (\alpha^2 x + x^2 - 2a^\lambda x^\lambda) = a^{2\lambda + 1} \left( 1 + \frac{1}{2\lambda + 1} - \frac{2}{\lambda + 1} \right) = \frac{2\lambda^2 a^{2\lambda + 1}}{2\lambda^2 + 3\lambda + 1} \]

We then extremize \( E \):

\[
\frac{dE}{d\lambda} \propto \frac{BdA - AdB}{B^2}
\]

where \( d\lambda = d/d\lambda \), gives

\[ BdA - AdB = 0 \]

Evaluating the derivatives using \( d\lambda e^{p\lambda + q} = d\lambda e^{(p\lambda + q)\ln a} = (p \ln a)e^{p\lambda + q} \) we have

\[ d\lambda A = \left( \frac{2}{\lambda} + 2 \ln a - \frac{2}{2\lambda - 1} \right) A \]

\[ d\lambda B = \left( \frac{2}{\lambda} + 2 \ln a - \frac{4\lambda + 3}{2\lambda^2 + 3\lambda + 1} \right) B \]

Putting it all together we get

\[ 4\lambda^2 - 4\lambda - 5 = 0 \rightarrow \lambda = \frac{1 + \sqrt{6}}{2} \]

This root gives the best answer; also the negative root gives a sharp cusp at the origin. The ground state estimate becomes

\[ E = -\frac{\hbar^2}{2m} A = -\frac{\hbar^2}{2m} \frac{2\lambda^2 + 3\lambda + 1}{2(2\lambda - 1)} \approx 2.4747 \frac{\hbar^2}{2ma^2} \]

The exact solution is \( \psi(x) = a^{-1/2} \cos (\pi x/2a) \) which gives

\[ -\frac{\hbar^2}{2m} \psi'' = \frac{\hbar^2}{2m} \frac{\pi^2}{4a^2} \psi \rightarrow E = \frac{\pi^2}{4} \frac{\hbar^2}{2ma^2} \approx 2.4674 \frac{\hbar^2}{2ma^2} \]

The agreement is very good and the variational estimate is greater than the ground state energy, as it must be.

### 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.

In the absence of coupling between the electron and proton spins, the appropriate quantum numbers are the uncoupled representation.

The ground state: 1s has degeneracy 4; up-down electron and up-down proton. We have quantum numbers:

\[ |n = 1, \ell = 0, m_\ell = 0, s = 1/2, i = 1/2, m_s, m_i \rangle \quad m_s = \pm 1/2, m_i = \pm 1/2 \]

(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 \( m_f \)?

Now include the hyperfine interaction. Let \( \vec{f} = \vec{i} + \vec{s} \) which is the total spin angular momentum. We note that

\[ f^2 = s^2 + i^2 + 2 \vec{s} \cdot \vec{i} \rightarrow \vec{s} \cdot \vec{i} = \frac{1}{2} (f^2 - s^2 - i^2) \]

This implies that the eigenstates of \( \hat{H}_{HF} \) are coupled \( \vec{s} \) and \( \vec{i} \), i.e., \( \{ f^2, s^2, i^2, f_z \} \) or the good quantum numbers are

\[ |n = 1, \ell = 0, s = 1/2, i = 1/2, f, m_f \rangle \]

The values of \( f \) range from \( |s - i| \leq f \leq s + i \). Therefore with \( s = i = 1/2 \) we have \( f = 0 \rightarrow m_f = 0 \) or \( f = 1 \rightarrow m_f = 1, 0, -1 \)

(c) The perturbed 1s ground state now has hyperfine splitting. The energy level diagram is sketched below.

![Figure 10.8: Hyperfine Splitting](image)

Label all the quantum numbers for the four sublevels shown in the figure.

(d) Show that the energy level splitting is

\[ \Delta E_{HF} = g_s g_i \mu_B \mu_N \langle \frac{1}{r^3} \rangle_1s \]

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Show numerically that this splitting gives rise to the famous 21 cm radio frequency radiation used in astrophysical observations.

Using

\[ \hat{f}^2 | m_f s i \rangle = f(f + 1) | m_f s i \rangle \]

\[ \hat{s}^2 | m_f s i \rangle = s(s + 1) | m_f s i \rangle = \frac{3}{4} | m_f s i \rangle \]

\[ \hat{i}^2 | m_f s i \rangle = i(i + 1) | m_f s i \rangle = \frac{3}{4} | m_f s i \rangle \]

we have

\[ \hat{s} \cdot \hat{i} | m_f s i \rangle = \frac{1}{2} \left( f(f + 1) - \frac{3}{2} \right) | m_f s i \rangle \]

so that

\[ f = 0 \rightarrow \hat{s} \cdot \hat{i} | 0, 0, 1/2, 1/2 \rangle = -\frac{3}{4} | 0, 0, 1/2, 1/2 \rangle \]

\[ f = 1 \rightarrow \hat{s} \cdot \hat{i} | 1, m_f, 1/2, 1/2 \rangle = +\frac{4}{4} | 1, m_f, 1/2, 1/2 \rangle \]

Therefore,

\[ E_{1s(f=0)} = -\frac{3}{4} g_s g_i \mu_B \mu_N \left\langle \frac{1}{r^3} \right\rangle_{\ell s} \]

\[ E_{1s(f=1)} = +\frac{1}{4} g_s g_i \mu_B \mu_N \left\langle \frac{1}{r^3} \right\rangle_{\ell s} \]

Thus,

\[ \Delta E_{HF} = E_{1s(f=1)} - E_{1s(f=0)} = g_s g_i \mu_B \mu_N \]

The level diagram is

![Level Diagram](image)

### 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?

The potential in the problem is \( V = 50(e^{-x} - 1)^2 \).
It is basically quadratic around zero and is very steep. One may guess that the harmonic oscillator is a pretty good approximation.

**Initial Guess:**

\[
\text{Initial Guess:} \\
\text{Series}[V, \{x, 0, 3\}] \\
50 \ x^2 - 50 \ x^3 + 6 \ x^4 \\
\]

If we try to identify the first term with the harmonic oscillator potential \(m \omega^2 x^2\), we find \(\omega = 10\) because \(m = 1\). Then one may hope that it would give the ground state energy \(\hbar \omega / 2 = 5\). However, this hope is not fulfilled. Using the ground state wave function of the harmonic oscillator,

\[
\psi_{1\text{raw}} = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} e^{-m \omega x^2 / (2 \hbar)} ; \\
\psi_1 = \psi_{1\text{raw}} / \{m \to 1, \omega \to 10, \hbar \to 1\} \\
e^{-5x^2} / \left( \frac{10}{\pi} \right)^{1/4}
\]

we compute the total energy using the Hamiltonian in the position space:
The error is

\[
\frac{N[Ebar1] - 39/8}{39/8} = 0.0722121
\]

and is bigger than 5%, but is pretty good, accurate within 7.22%. Therefore, we are motivated to try a non-SHO Gaussian as a trial function.

**Gaussian Trial Function**:

\[
\psi_2 = \frac{1}{\pi^{1/4} \Delta^{1/2}} e^{-\psi^2/(2\Delta)};
\]

\[
K2 = -\frac{\hbar^2}{2m} \text{Integrate}[\psi_2 D(\psi_2, \{x, 2\}), \{x, -\infty, \infty\}, \text{Assumptions} \rightarrow \Delta > 0] / \{n \rightarrow 1, m \rightarrow 1\}
\]

\[
P2 = \text{Integrate}[\psi_2^2 V, \{x, -\infty, \infty\}, \text{Assumptions} \rightarrow \Delta > 0]
\]

\[
Ebar2 = K2 + P2
\]

\[
Ebar2_{\text{min}} = \text{FindMinimum}[Ebar2, \{\Delta, 10^{-1/3}\}]
\]

\{5.20891, \{\Delta \rightarrow 0.304036\}\}
It has improved, but is not yet within 5%.

**Linear times Gaussian**: One way to improve it further is the following. Note that the potential is not parity symmetric, and hence the ground state wavefunction is not expected to be an even function. Because the potential is lower on the right, we expect the wave function is skewed towards the right. Therefore, we can try

$$
\psi_3 = (1 + k x) e^{-x^2/(2 \lambda^2)} ;
$$

It is not normalized at this point, and we calculate its norm

\[
\text{norm3} = \text{Integrate}[\psi^2, \{x, -\infty, \infty\}, \text{Assumptions} \to \lambda > 0] \\
\frac{1}{2} \sqrt{\pi \lambda} \left(2 + k^2 \lambda^2\right)
\]

\[
K_3 = \frac{-\lambda^2}{2} \text{Integrate}[\psi_3 \partial \psi_3, \{x, -\infty, \infty\}, \text{Assumptions} \to \lambda > 0] / \lambda (m+1, n-1) \\
\frac{\sqrt{\pi}}{8 \lambda} \left(2 + 3 k^2 \lambda^2\right)
\]

\[
P_3 = \text{Integrate}\left[\psi_3 \nabla \psi_3, \{x, -\infty, \infty\}, \text{Assumptions} \to \lambda > 0\right] \\
25 \sqrt{\pi} \lambda \left[2 k^2 \lambda^2 - e^{\lambda^2} \left(2 - k^2 \lambda^2\right) \left(-4 - k^2 \lambda^2\right)\right] - e^{\lambda^2} \left(4 + k^2 \lambda^2\right) \left(-4 + k^2 \lambda^2\right)
\]

\[
\text{Ebar3} = \frac{K_3 \cdot P_3}{\text{norm3}} \\
\frac{1}{2 \sqrt{\pi} \lambda \left(2 + k^2 \lambda^2\right)} \left[2 \sqrt{\pi} \lambda \left(2 + 3 k^2 \lambda^2\right) - 25 \sqrt{\pi} \lambda \left[2 k^2 \lambda^2 - e^{\lambda^2} \left(2 - k^2 \lambda^2\right) \left(-4 - k^2 \lambda^2\right)\right] - e^{\lambda^2} \left(4 + k^2 \lambda^2\right) \left(-4 + k^2 \lambda^2\right)\right]
\]

\[
\text{Ebarmin} = \text{FindMinimum}[\text{Ebar3}, \{\lambda, 10^{0.5}\}, \{k, 0\}]
\]

\[
(4.92619, \{\lambda \to 0.331105, k \to 0.764297\})
\]

\[
\text{Ebarmin}[[1]] - 39 / 8 \\
39 / 8
\]

This is correct at the 1% level! The wave function is therefore
As expected, it is more or less a Gaussian, but skewed to the right.

**The Analytic Solution:** This problem is actually a special case of the Morse potential

\[ V_m = D \left( e^{-a u} - 1 \right)^2 \]

This potential is a form of the inter-atomic potential in diatomic molecules proposed by P.M. Morse, *Phys. Rev.* **34**, 57 (1929). The variable \( u \) is the distance between the two atoms minus its equilibrium distance \( u = r - r_0 \). The Schrödinger equation can be solved analytically. Expanding it around the minimum,

\[
\text{Series}[V_m, \{u, 0, 4\}] = a^4 \Delta u^4 - a^4 \Delta u^3 - \frac{7}{12} a^4 \Delta u^2 + O[u]^3
\]

The harmonic oscillator approximation gives \( \omega = \sqrt{2a^2D/m} \). The correct energy eigenvalues are known to be

\[
E_n = \hbar \omega \left( n + \frac{1}{2} \right) - \frac{\hbar^2 a^2}{2m} \left( n + \frac{1}{2} \right)^2
\]

where the second term is called the anharmonic correction. For large \( n \), the second term will dominate and the energy appears to become negative. Clearly, the bound state spectrum does not go on forever, and ends at a certain value of \( n \), quite different from the harmonic oscillator. But this is expected because the potential energy asymptotes to \( D \) for \( u \to +\infty \) and hence states for \( E > D \)
must be unbound and have a continuous spectrum.

The ground state wave function is known to have the form

$$\psi_m = E^{-d} e^{-u} e^{-b a/2}$$

where \( b = 2d - 1 \), \( d = \sqrt{2Dm/\hbar} \). Let us see that it satisfies the Schrodinger equation.

The first term is \( \hbar \omega / 2 = \hbar a \sqrt{D/2M} \) and the zero-point energy with the harmonic oscillator approximation. The second term \( -\hbar^2 a^2 / 8m \) is the anharmonic correction.

The normalization is

$$\frac{2^{-d} \Gamma(b)}{a}$$

Actually, this wave function could have been guessed if one pays a careful attention to the asymptotic behaviors. For \( u \to \infty \), the potential asymptote to \( D \) and hence the wave function must damp exponentially as \( e^{-\kappa u} \) with \( \kappa = \sqrt{2m|E|/\hbar} \). For \( u \to -\infty \), the potential rises extremely steeply as \( De^{-2au} \). It suggests that the energy eigenvalue becomes quickly irrelevant and the behavior of the wave function must be given purely by the rising behavior of the potential. By dropping the energy eigenvalue and looking at the Schrodinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{du^2} + D e^{-2au} \psi = 0$$

and change the variable to \( y = e^{-au} \psi \). we find

$$-\frac{\hbar^2}{2m} \left( \frac{d^2 \psi}{dy^2} + \frac{1}{y} \frac{d \psi}{dy} \right) + D \psi = 0$$

The second term in the parentheses is negligible for \( y \to \infty \). Therefore the wave function has the behavior

$$\psi \propto e^{-\sqrt{2mDy/\hbar}}$$
Combining the behavior on both ends, the wave function has precisely the exact form given above. This is the lesson: the one-dimensional potential problem is so simple that there are many ways to study the behavior of the wave function. On the other hand, the real-world problem involves many more degrees of freedom. In many cases, the Hamiltonian itself must be guessed.

Back to the Morse potential. The case in this problem has $D = 50$, $a = 1$, $m = 1$, $\hbar = 1$. Therefore, the ground state energy is

$$E_0 = \frac{1}{2} \hbar a \sqrt{\frac{D}{2m}} - \frac{\hbar^2 a^2}{8m} = 5 - \frac{1}{8} = \frac{39}{8}$$

```
ψmf = Simplify[1/Sqrt[Morse2a] \[ψ[m, \{b -> 2 d - 1\} /. \{d -> \[Sqrt][2 D m]/a \[hbar\}\} /. \{D -> 50, a -> 1, m -> 1, \[hbar] -> 1\}]
```

```
567.5
```

Plot[ψmf, {u, -1, 1}, PlotPoints -> 50];
The variational linear time Gaussian wave function was quite close.

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,

$$ - \frac{p^4}{8m_e^3c^2} + g \frac{1}{4m_e^2c^2} \frac{1}{r} \frac{dV_c}{dr}(\vec{L} \cdot \vec{S}) + \frac{\hbar^2}{8m_e^2c^2} \nabla^2 V_c, \quad V_c = -\frac{Ze^2}{r} $$

Quite close.
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.

**Preliminaries:** We use the 2s wave function

\[
R_{2s} = (2a)^{-3/2} \left( 2 - \frac{r}{a} \right) e^{-r/(2a)};
\]

The full wave function is

\[
\Psi_{2s} = \frac{1}{\sqrt{4\pi}} R_{2s};
\]

Here, \( a = a_0/Z = \hbar^2/(Ze^2m) \). Similarly,

\[
R_{2p} = (2a)^{-3/2} \frac{r}{\sqrt{3a}} e^{-r/(2a)};
\]

As a preparation for calculating the spin-orbit interaction, we have

\[
\vec{L} \cdot \vec{S} = \frac{1}{2}(J^2 - L^2 - S^2) = \frac{\hbar^2}{2}(j(j + 1) - \ell(\ell + 1) - s(s + 1))
\]

For \( j = \ell + 1/2 \),

\[
\vec{L} \cdot \vec{S} = \frac{\hbar^2}{2}((\ell + 1/2)(\ell + 3/2) - \ell(\ell + 1) - 3/4) = \frac{\hbar^2}{2}\ell
\]

For \( j = \ell - 1/2 \),

\[
\vec{L} \cdot \vec{S} = \frac{\hbar^2}{2}((\ell - 1/2)(\ell + 1/2) - \ell(\ell + 1) - 3/4) = -\frac{\hbar^2}{2}(\ell + 1)
\]

For the calculations of the relativistic corrections, we use the fact that

\[
- \frac{\hbar^4}{8m^3c^2} (\rho^4) = -\frac{1}{8m^3c^2} (\langle -\hbar^2 \nabla^2 \rangle^2)
\]

\[
\frac{1}{8m^3c^2} \int d^3x \psi^* \nabla^4 \psi = -\frac{1}{8m^3c^2} \int d^3x (\nabla^2 \psi)^*(\nabla^2 \psi)
\]

\[
- \frac{1}{8m^3c^2} \int d^3x \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell + 1)}{r^2} \right) (RY_{\ell m}^m)^* \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell + 1)}{r^2} \right) (RY_{\ell m})
\]

\[
- \frac{1}{8m^3c^2} \int r^2 dr \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell + 1)}{r^2} \right) R(r) \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell + 1)}{r^2} \right) R(r)
\]

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The Darwin term for the Coulomb potential is proportional to

$$\Delta V_c = \nabla^2 \left( -\frac{Z e^2}{r} \right) = 4\pi Z e^2 \delta(\vec{x}) = 4\pi \frac{\hbar^2}{ma} \delta(\vec{x})$$

2s: First the relativistic correction

$$\int \left[ -\frac{2}{8 m^3 c^2} \left( D[R_{s}, \{r, 2\}] + \frac{2}{r} D[R_{s}, r] \right) r^2, \{r, 0, \infty\}, \text{Assumptions} \rightarrow a > 0 \right]$$

$$= \frac{13 \hbar^4}{128 a^4 c^2 m^3}$$

Second, the spin-orbit interaction. Because $L = 0$, it identically vanishes. Third, the Darwin term.

$$\frac{\hbar^2}{8 m^2 c^2} - 4\pi \frac{\hbar^2}{ma} \psi_{2s}^2 / \{r \rightarrow 0\}$$

$$\frac{\hbar^4}{16 a^4 c^2 m^3}$$

2p$_{1/2}$: For the relativistic correction

$$\int \left[ -\frac{\hbar^4}{8 m^3 c^2} \left( D[R_{2p}, \{r, 2\}] + \frac{2}{r} D[R_{2p}, r] - \frac{2}{r^2} R_{2p} \right) r^2, \{r, 0, \infty\}, \text{Assumptions} \rightarrow a > 0 \right]$$

$$= \frac{7 \hbar^4}{384 a^4 c^2 m^3}$$

Second, the spin-orbit interaction.

$$\int \left[ -\frac{g}{4 m^2 c^2} \frac{1}{r^3} \frac{\hbar^2}{ma} (-\hbar^2) R_{2p}^2 r^2, \{r, 0, \infty\}, \text{Assumptions} \rightarrow a > 0 \right]$$

$$= \frac{g \hbar^5}{96 a^4 c^2 m^3}$$
Third, the Darwin term. Because the wave function vanishes at the origin, it is identically zero.

\[ \psi \psi / \{ g \rightarrow 2 \} \]

\[ - \frac{5 \hbar^4}{128 a^4 c^2 m^3} \]

### $2p_{3/2}$

First, the relativistic correction. We use the fact that

\[ p^2 \psi = -\hbar^2 \nabla^2 \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{2}{r^2} \right) R(r) \]

\[
\text{Integrate} \left[ -\frac{\hbar^4}{8 m^2 c^2} \left( D[R_{2p}, \{ r, 2 \}] + \frac{2}{r} D[R_{2p}, r] - \frac{2}{r^2} R_{2p} \right)^2 \right] \quad \text{\{r, 0, \infty\}, Assumptions \rightarrow a > 0} \\
- \frac{7 \hbar^4}{384 a^4 c^2 m^3} \]

Second, the spin-orbit interaction.

\[
\text{Integrate} \left[ \frac{g \hbar^4}{4 m^2 c^2} \frac{1}{r^3} \frac{\hbar^2}{m a} \frac{\hbar^2}{2} R_{2p}^2 r^2, \{ r, 0, \infty\}, Assumptions \rightarrow a > 0 \right] \\
- \frac{g \hbar^4}{192 a^4 c^2 m^3} \]

Third, the Darwin term. Because the wave function vanishes at the origin, it is identically zero.

\[ \psi \psi / \{ g \rightarrow 2 \} \]

\[ - \frac{\hbar^4}{128 a^4 c^2 m^3} \]

### Summary

Therefore, the $2s$ and $2p_{1/2}$ states are still degenerate, and have the energy

\[ -\frac{e^2}{8a} - \frac{5\hbar^4}{128a^4 m^3 c^2} = -\frac{e^2}{a} \left( \frac{1}{8} + \frac{5}{128} \alpha^2 \right) \]

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while the $2p_{3/2}$ states have the energy

$$-\frac{e^2}{a} \left( \frac{1}{8} + \frac{1}{128} a^2 \right)$$

where $a = e^3/\hbar c$. Numerically, (we took $g = 2$ above for comparison between $2s$ and $2p$), the energy shifts in $eV$ are

$\begin{align*}
\text{constants} &= \{ e \rightarrow 1.60217663 \times 10^{-19}, \frac{5}{2}, 9.29725 \times 10^{-5}, \text{a} \rightarrow 1.291772108 \times 10^{-9}, \text{a} \rightarrow 1 / 137.03599911 \}; \\
\text{ergtoev} &= 6.241506 \times 10^{14} ; \\
-\frac{e^2}{a} \left( \frac{5}{128} a^2 \right) &/ . \text{constants} \ast \text{ergtoev} \\
-\frac{e^2}{a} \left( \frac{1}{128} a^2 \right) &/ . \text{constants} \ast \text{ergtoev} \\
\text{ OUTPUT} &= \begin{cases} \\
-0.0000566032 \\
-0.0000113206 \\
0.000452826 \\
\end{cases}
\end{align*}$

### 10.9.48 Hyperfine Interaction Again

Show that the interaction between two magnetic moments is given by the Hamiltonian

$$H = -\frac{2}{3} \mu_0 (\vec{\mu}_1 \cdot \vec{\mu}_2) \delta(\vec{z} - \vec{y}) - \frac{\mu_0}{4\pi \alpha^3} \left( 3 \frac{r_i r_j}{r^2} \right) \mu_1 \mu_2$$

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?

We start with Maxwell’s equations

$$\begin{align*}
\nabla \cdot \vec{E} &= 4\pi \rho \\
\nabla \times \vec{B} &= \frac{1}{c} \vec{j} + \frac{4\pi}{c} \vec{E} \\
\nabla \times \vec{E} &= -\frac{1}{c} \vec{B} \\
\nabla \cdot \vec{B} &= 0
\end{align*}$$

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They are derived from the action

\[ S = \int dt d^3x \left( \frac{1}{8\pi} (E^2 + B^2) - \phi \rho + \frac{1}{c} A \cdot j \right) \]

A magnetic moment couples to the magnetic field with the Hamiltonian \( H = -\vec{\mu} \cdot \vec{B} \), and therefore appears in the Lagrangian as \( L = +\vec{\mu} \cdot \vec{B} \). We add this term to the above action

\[ S = \int dt d^3x \left( \frac{1}{8\pi} (E^2 + B^2) - \phi \rho + \frac{1}{c} \vec{A} \cdot \vec{j} + \vec{\mu} \cdot \vec{B} \delta(\vec{x} - \vec{y}) \right) \]

where \( \vec{y} \) is the position of the magnetic moment. The equation of motion for the vector potential is obtained by varying the action with respect to \( \vec{A} \),

\[ \nabla \times \vec{B} = \frac{1}{c} \dot{\vec{E}} + \frac{4\pi}{c} \vec{j} - 4\pi \vec{\mu} \times \nabla \delta(\vec{x} - \vec{y}) \]

In the absence of time-varying electric field or electric current, the equations is simply

\[ \nabla \times \vec{B} = -4\pi \vec{\mu} \times \nabla \delta(\vec{x} - \vec{y}) \]

It is tempting to solve it immediately as

\[ \vec{B} = -\vec{\mu} \delta(\vec{x} - \vec{y}) \]

but this misses possible terms of the form \( \vec{B} \propto \nabla f \) where \( f \) is a scalar function.

To solve it, we use the Coulomb gauge and write the equation of motion as

\[ \nabla^2 \vec{A} = -4\pi \vec{\mu} \times \nabla \delta(\vec{x} - \vec{y}) \]

Because

\[ \nabla \frac{1}{|\vec{x} - \vec{y}|} = -4\pi \delta(\vec{x} - \vec{y}) \]

we find

\[ \vec{A}(\vec{x}) = -\vec{\mu} \times \nabla \frac{1}{|\vec{x} - \vec{y}|} = \vec{\mu} \times \frac{\vec{x} - \vec{y}}{|\vec{x} - \vec{y}|^2} \]

The magnetic field is its curl,

\[ \vec{B} = \nabla \times \vec{A} = -\vec{\mu} \nabla^2 \frac{1}{|\vec{x} - \vec{y}|} + \nabla (\vec{\mu} \cdot \nabla) \frac{1}{|\vec{x} - \vec{y}|} \]

We rewrite the latter term as

\[ \nabla_i \nabla_j = \left( \nabla_i \nabla_j - \frac{1}{3} \vec{\mu} \nabla^2 \right) + \frac{1}{3} \delta_{ij} \nabla^2 \]

so that the terms in the parentheses averages out for an isotropic source. They are called the tensor term while the latter the scalar term. Then

\[ \vec{B} = \nabla \times \vec{A} = \frac{2}{3} \vec{\mu} \nabla^2 \frac{1}{|\vec{x} - \vec{y}|} + \left( \nabla (\vec{\mu} \cdot \nabla) - \frac{1}{3} \vec{\mu} \nabla^2 \right) \frac{1}{|\vec{x} - \vec{y}|} \]
After doing the differentiation, we have
\[ \vec{B} = \frac{8\pi}{3} \vec{\mu} \delta(\vec{x} - \vec{y}) + \frac{1}{r^3} \left( 3 \frac{\vec{r} \cdot \vec{\mu}}{r} \frac{\vec{r}}{r} - \vec{\mu} \right) \]
where we used \( \vec{r} = \vec{x} - \vec{y} \).

Finally, the interaction of two magnetic moments, \( \vec{\mu}_1 \) at \( \vec{x} \) and \( \vec{\mu}_2 \) at \( \vec{y} \), is given by the magnetic field created by the second magnetic moment at \( \vec{y} \)
\[ H = -\vec{\mu}_1 \cdot \vec{B}(\vec{x}) = -\frac{8\pi}{3} \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 \delta(\vec{x} - \vec{y})}{r^3} \left( 3 \frac{\vec{r} \cdot \vec{\mu}_1 \vec{r}}{r} - \vec{\mu}_1 \cdot \vec{\mu}_2 \right) \]
In the MKSA system, it is
\[ H = -\vec{\mu}_1 \cdot \vec{B}(\vec{x}) = -\frac{2\mu_0}{3} \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 \delta(\vec{x} - \vec{y})}{4\pi r^3} \left( 3 \frac{\vec{r} \cdot \vec{\mu}_1 \vec{r}}{r} - \vec{\mu}_1 \cdot \vec{\mu}_2 \right) \]
For hyperfine splittings in the 1s state of the hydrogen atom (\( Z = 1 \)), the second term vanishes because it is a spherical tensor with \( q = 2 \), and hence only the first term is needed. The magnetic moments are (in MKSA)
\[ \vec{\mu}_e = g_e \frac{e}{2m_e} \vec{s}_e \quad , \quad \vec{\mu}_p = g_p \frac{e}{2m_p} \vec{s}_p \]
where \( g_e = 2 \) and \( g_p = 2.79 \times 2 \). It is useful to define
\[ \mu_e = \frac{|e|\hbar}{2m_e} \quad , \quad \mu_N = \frac{|e|\hbar}{2m_p} \]
and
\[ \vec{\mu}_e = g_e \mu_e \frac{2 \vec{s}_e}{\hbar} \quad , \quad \vec{\mu}_p = 2.79 \mu_N \frac{2 \vec{s}_p}{\hbar} \]
Therefore, the Hamiltonian is
\[ H = +\frac{2\mu_0}{3} \frac{2.79\mu_N \mu_e}{4 \hbar^2} (\vec{s}_p \cdot \vec{s}_e) \delta(\vec{x}) \]
The first order perturbation of this Hamiltonian gives the hyperfine splitting
\[ E_{ff} = +\frac{2\mu_0}{3} \frac{2.79\mu_N \mu_e}{4 \hbar^2} (\vec{s}_p \cdot \vec{s}_e) |\psi(0)|^2 \]
with \( |\psi(0)|^2 = 1/(\pi a_0^3) \) for the 1s state. Finally, the eigenvalues of the spin operators are
\[ \vec{s}_p \cdot \vec{s}_e \frac{1}{2} ((\vec{s}_p + \vec{s}_e))^2 - \vec{s}_p^2 - \vec{s}_e^2 = \begin{cases} \frac{\hbar^2}{4} & F = 1 \\ -\frac{3\hbar^2}{4} & F = 0 \end{cases} \]
Therefore, the difference in energies is
\[
\Delta E = \frac{2\mu_0 2.79\mu_N\mu_e}{3} \frac{4}{\hbar^2} \left( \frac{\hbar^2}{4} - \left( -\frac{3\hbar^2}{4} \right) \right)
= \frac{2\mu_0 2.79\mu_N\mu_e}{3} \frac{4}{\pi a_0^3} = 9.39 \times 10^{-25} \text{ J}
\]

Parametrically, it is \( \alpha^2 (m/\mu_p) \) times the binding energy and hence even more suppressed than the fine structure.

The cosmic thermal bath has \( T = 2.7^\circ \text{K} \) and hence \( kT = 3.7 \times 10^{-23} \text{ J} \), which is much larger than the hyperfine splitting.

The deexcitation of the \( F = 1 \) states to the \( F = 0 \) state emits a photon of the wavelength 21 cm, and it is called the 21 cm line. It has had an important impact on astronomy. Because the wavelength is much longer than typical dust particles, it can be seen through the dust which blocks photons in the optical range. Because the cosmic thermal bath is hot enough to excite the hydrogen to the \( F = 1 \) states, we can see the 21 cm lines even from the region without stars and hot gas. Namely any hydrogen gas emits the 21 cm line. For instance, the spiral arms in our Milky Way galaxy had been discovered using the 21 cm line. Its frequency is 1420.4058 MHz, and hence in the radio range.

### 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 \( B = B\hat{z} \) and have the same gyromagnetic ratio \( \gamma \).

(a) Determine the energy eigenvalues and eigenstates for \( H_0 \)

It is easy to intuit,
\[
\begin{align*}
|+z\rangle_A \otimes |+z\rangle_B & \quad E_{++} = \hbar \omega_L \\
|+z\rangle_A \otimes |-z\rangle_B & \quad E_{+-} = 0 \\
|-z\rangle_A \otimes |+z\rangle_B & \quad E_{-+} = 0 \\
|-z\rangle_A \otimes |-z\rangle_B & \quad E_{--} = -\hbar \omega_L
\end{align*}
\]
where \( \omega_L = -\gamma B_z \) and the factors on \( H_A \) and \( H_B \) are eigenstates of \( S_z^A \) and \( S_z^B \).
(b) Suppose we now add a perturbation term \( H_{\text{total}} = H_0 + W \), 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.

The corrections for \( E_{++} \) and \( E_{--} \) are easy to compute since these are non-degenerate eigenvalues:
\[
E_{++} \rightarrow E_{++} + \langle ++|W|++\rangle = \hbar \omega_L + \lambda \frac{\hbar \omega}{4}
\]
\[
E_{--} \rightarrow E_{--} + \langle --|W|--\rangle = -\hbar \omega_L + \lambda \frac{\hbar \omega}{4}
\]

For \( E_{+-} \) and \( E_{-+} \), we need to diagonalize the restriction of \( W \) on the corresponding subspace. The matrix representation of this restriction is
\[
W_0 \leftrightarrow \left( \begin{array}{c}
\langle ++|W|+-\rangle \\
\langle --|W|+-\rangle \\
\langle ++|W|-+\rangle \\
\langle --|W|-+\rangle
\end{array} \right)
\]

and to compute it we first derive the matrix representation of \( W \) on the entire joint Hilbert space. Using the rules for tensor products of matrices,
\[
S_x^A \otimes S_x^B \leftrightarrow \frac{\hbar^2}{4} \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix},
S_y^A \otimes S_y^B \leftrightarrow \frac{\hbar^2}{4} \begin{pmatrix}
0 & 0 & 0 & -1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0
\end{pmatrix}
\]
\[
S_z^A \otimes S_z^B \leftrightarrow \frac{\hbar^2}{4} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix},
W \leftrightarrow \lambda \frac{\hbar^2}{4} \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 2 & 0 \\
0 & 2 & -1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

With the corresponding vector representations of \( |+-\rangle \) and \( |--\rangle \),
\[
|+-\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix},
|--\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\]

we have
\[
\langle ++|W|--\rangle = \lambda \frac{\hbar^2}{2},
\langle --|W|++\rangle = \lambda \frac{\hbar^2}{2}
\]
\[
\langle ++|W|+-\rangle = \lambda \frac{\hbar^2}{2},
\langle --|W|-+\rangle = -\lambda \frac{\hbar^2}{2}
\]

So in the end
\[
W_0 \leftrightarrow \lambda \frac{\hbar^2}{4} \begin{pmatrix}
-1 & 2 & 0 \\
2 & -1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]
The eigenvalue equation is

\((-1 - \epsilon)^2 - 4 = 0 \rightarrow \epsilon + 1 = \pm 2\)

so

\[\epsilon = \left\{ \frac{\hbar^2}{4}, -3\frac{\hbar^2}{4} \right\}\]

and the corresponding eigenvectors are determined by

\[
\begin{pmatrix}
-2 & 2 \\
2 & -2
\end{pmatrix}
\begin{pmatrix}
a \\
b
\end{pmatrix} = 0 \rightarrow \begin{pmatrix} a \\ b \end{pmatrix} \propto \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\]

and

\[
\begin{pmatrix}
2 & 2 \\
2 & 2
\end{pmatrix}
\begin{pmatrix}
a \\
b
\end{pmatrix} = 0 \rightarrow \begin{pmatrix} a \\ b \end{pmatrix} \propto \begin{pmatrix} 1 \\ -1 \end{pmatrix}
\]

and so the proper zeroth-order states in the degenerate subspace for \(H_0\) are

\[|W_+\rangle = \frac{1}{\sqrt{2}}(|++\rangle + |--\rangle), \quad |W_-\rangle = \frac{1}{\sqrt{2}}(|++\rangle - |--\rangle)\]

with corresponding energy corrections

\[\langle W_+ | W_0 | W_+ \rangle = \frac{\hbar^2}{4}, \quad \langle W_- | W_0 | W_- \rangle = -3\frac{\hbar^2}{4}\]

Finally, the first-order energy corrections are

\[\{\hbar \omega_L, 0, 0, -\hbar \omega_L\} \rightarrow \left\{ \hbar \omega_L + \frac{\lambda \hbar^2}{4}, \frac{3\lambda \hbar^2}{4}, -3\lambda \hbar^2, -\hbar \omega_L - 3\lambda \hbar^2 \right\}\]

### 10.9.50 More Perturbation Practice

Consider two spin-1/2 degrees of freedom, whose joint pure states can be represented by state vectors in the tensor-product Hilbert space \(H_{AB} = H_A \otimes H_B\), where \(H_A\) and \(H_B\) are each two-dimensional. Suppose that the initial Hamiltonian for the spins is

\[H_0 = (-\gamma_A B_z S_z^A) \otimes I^B + I^A \otimes (-\gamma_B B_z S_z^B)\]

(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.

The eigenstates are clearly \(\{|+a+b\rangle, |+a-b\rangle, |-a+b\rangle, |-a-b\rangle\}\), with corresponding energies

\[H_0 |+a+b\rangle = \frac{\hbar}{2}(-\gamma_a - \gamma_b)B_z\]
\[H_0 |+a-b\rangle = \frac{\hbar}{2}(-\gamma_a + \gamma_b)B_z\]
\[H_0 |-a+b\rangle = \frac{\hbar}{2}(\gamma_a - \gamma_b)B_z\]
\[H_0 |-a-b\rangle = \frac{\hbar}{2}(\gamma_a + \gamma_b)B_z\]
If $\gamma_a \neq \gamma_b$ and $\gamma_a, \gamma_b \neq 0$ these eigenenergies are non-degenerate.

(b) Compute the first-order corrections to the eigenstates under the perturbation

$$W = \alpha S_A^x \otimes S_B^x$$

where $\alpha$ is a small parameter with appropriate units.

We use the general formula

$$\lambda |1\rangle = \sum_{p \neq n} \frac{\langle \phi_p | W | \phi_n \rangle}{E_n^0 - E_p^0} |\phi_p\rangle$$

and note that

$$S_A^x \otimes S_B^x |+a+b\rangle = \frac{\hbar^2}{4} |\pm a-b\rangle$$
$$S_A^x \otimes S_B^x |+a-b\rangle = \frac{\hbar^2}{4} |\pm a+b\rangle$$
$$S_A^x \otimes S_B^x |-a+b\rangle = \frac{\hbar^2}{4} |\pm a-b\rangle$$
$$S_A^x \otimes S_B^x |-a-b\rangle = \frac{\hbar^2}{4} |\pm a+b\rangle$$

For the $|+a+b\rangle$ state,

$$\lambda |1\rangle \rightarrow -\frac{\hbar^2}{4} \frac{\langle -a-b | W | +a+b \rangle}{\hbar(\gamma_a + \gamma_b)B_z} = -\frac{h\alpha}{4(\gamma_a + \gamma_b)B_z} |\pm a-b\rangle$$

Similarly, for the $|+a-b\rangle$ state

$$\lambda |1\rangle \rightarrow -\frac{\hbar^2}{4} \frac{\langle -a+b | W | +a-b \rangle}{\hbar(-\gamma_a + \gamma_b)B_z} = -\frac{h\alpha}{4(\gamma_a - \gamma_b)B_z} |\pm a+b\rangle$$

For the $|-a+b\rangle$ state,

$$\lambda |1\rangle \rightarrow \frac{\hbar^2}{4} \frac{\langle +a-b | W | -a+b \rangle}{\hbar(\gamma_a - \gamma_b)B_z} = \frac{h\alpha}{4(\gamma_a - \gamma_b)B_z} |\pm a-b\rangle$$

and for the $|-a-b\rangle$ state,

$$\lambda |1\rangle \rightarrow -\frac{\hbar^2}{4} \frac{\langle +a+b | W | -a-b \rangle}{\hbar(\gamma_a + \gamma_b)B_z} = \frac{h\alpha}{4(\gamma_a + \gamma_b)B_z} |\pm a+b\rangle$$
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 \( \tau \) 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 \( t > \tau \).

In the \( n = 1 \) state of this potential well, the electron has these wave functions and corresponding energies

\[
\psi_n(x) = \sqrt{\frac{2}{a}} \sin \left( \frac{\pi n}{a} \left( \frac{a}{2} + x \right) \right) , \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}
\]

The uniform electric field \( \varepsilon \hat{e}_x \) has a potential energy

\[
H' = -(-e) \int \varepsilon dx = e \varepsilon x
\]
which we use a perturbation. We then have

\[ H'_{n_1n_2} = \langle n_1 | H' | n_2 \rangle = \frac{e\varepsilon}{a} \int_{-a/2}^{a/2} \sin \left( \frac{\pi n_1}{a} \left( \frac{a}{2} + x \right) \right) \sin \left( \frac{\pi n_2}{a} \left( \frac{a}{2} + x \right) \right) dx \]

\[ = \frac{e\varepsilon}{a} \int_{-a/2}^{a/2} \left[ \cos \left( \frac{\pi (n_1 - n_2)}{a} \left( \frac{a}{2} + x \right) \right) - \cos \left( \frac{\pi (n_1 + n_2)}{a} \left( \frac{a}{2} + x \right) \right) \right] dx \]

\[ = \frac{e\varepsilon a^2}{\pi^2 (n_1 - n_2)^2} \left[ (-1)^{n_1-n_2} - 1 \right] - \frac{a^2}{(n_1 + n_2)^2} \left[ (-1)^{n_1+n_2} - 1 \right] \]

since

\[ ((-1)^{n_1+n_2} - 1) = ((-1)^{n_1-n_2} - 1) \]

for all \( n_1, n_2 \). We also define

\[ \omega_{n_1n_2} = \frac{E_{n_2} - E_{n_1}}{\hbar} = \frac{\hbar \pi^2}{2ma^2} (n_2^2 - n_1^2) \]

Now, in time-dependent perturbation theory the amplitude for the transition \( q \rightarrow p \) is given by

\[ C_{pq}(t) = \frac{1}{i\hbar} \int_0^\tau H'_{pq} e^{i\omega_{pq} t} dt = \frac{1}{i\hbar \omega_{pq}} H'_{pq} \left( 1 - e^{i\omega_{pq} t} \right) \]

when \( H'_{pq} \) is time-independent. For the transition \( 1 \rightarrow 2 \) we have

\[ H'_{21} = \frac{4e\varepsilon a}{\pi^2} \frac{2}{9} (-2) = -\frac{16e\varepsilon a}{9\pi^2}, \quad \omega_{21} = \frac{3\hbar \pi^2}{2ma^2} \]

so that the probability finding the electron in the \( n = 2 \) state at \( t > \tau \) is

\[ P_2(t > \tau) = |C_{21}(t)|^2 = \frac{1}{h^2 \omega_{21}^2} H'_{21}^2 \left( 1 - e^{i\omega_{pq} t} \right) \left( 1 - e^{-i\omega_{pq} t} \right) \]

\[ = \frac{1}{\hbar^2 \left( \frac{3\hbar \pi^2}{2ma^2} \right)^2} \left( \frac{16e\varepsilon a}{9\pi^2} \right)^2 \left( 2 - 2 \cos \frac{3\hbar \pi^2}{2ma^2} t \right) \]

\[ = \frac{4m^2a^4}{9\hbar^4 \pi^4} \frac{256e\varepsilon^2 a^2}{81\pi^2} - 4 \sin^2 \frac{3\hbar \pi^2}{4ma^2} t = \frac{4m^2a^4 e^2 \varepsilon^2}{36\hbar^4 \pi^4} - \frac{4m^2a^4 e^2 \varepsilon^2}{36\hbar^4 \pi^4} \sin^2 \frac{3\hbar \pi^2}{4ma^2} t \]

For small \( \tau \)

\[ P_2(t > \tau) = \frac{4^6m^2a^6 e^2 \varepsilon^2}{3^6\hbar^4 \pi^4} \left( \frac{3\hbar \pi^2}{4ma^2} \right)^2 = \frac{4^4a^2 e^2 \varepsilon^2}{3^4\hbar^2 \pi^2} \tau^2 \]

For the transition \( 1 \rightarrow 3 \) we have

\[ H'_{31} = 0 \rightarrow P_3(t > \tau) = |C_{31}(t)|^2 = 0 \]

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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

$$V(x, y, z) = k (x^2 + y^2 + z^2)$$

(a) Find the three lowest energy levels $E_0$, $E_1$, $E_2$ and their associated degeneracy.

Using Cartesian coordinates

$$E_N = E_n + E_{\ell} + E_m = \frac{3}{2} \hbar \omega + (n + \ell + m) \hbar \omega = \frac{3}{2} \hbar \omega + N \hbar \omega$$

Therefore,

$$E_0 = \frac{3}{2} \hbar \omega = \frac{3}{2} \hbar \sqrt{\frac{2k}{M}} \rightarrow \text{non-degenerate } \psi_{000}$$

$$E_1 = \frac{5}{2} \hbar \omega = \frac{5}{2} \hbar \sqrt{\frac{2k}{M}} \rightarrow 3 \text{-fold degenerate } \psi_{100}, \psi_{010}, \psi_{001}$$

$$E_2 = \frac{7}{2} \hbar \omega = \frac{7}{2} \hbar \sqrt{\frac{2k}{M}} \rightarrow 6 \text{-fold degenerate } \psi_{200}, \psi_{020}, \psi_{002}, \psi_{110}, \psi_{101}, \psi_{011}$$

(b) Suppose a small perturbing potential $Ax \cos \omega t$ 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.

At time $t = 0$, $H' = Ax \cos \omega t$. The first order perturbation correction gives with $\ell$ being the quantum number for the component oscillator along the $x$-axis

$$\langle \ell' m' n' | H'(x, t) | \ell m n \rangle = \delta_{m' m} \delta_{n' n} \langle \ell' | H'(x, t) | \ell \rangle = A \alpha \cos \omega t \delta_{m' m} \delta_{n' n} \left[ \sqrt{\ell + 1} \delta_{\ell', \ell + 1} + \sqrt{\ell} \delta_{\ell', \ell - 1} \right]$$

where

$$\alpha = \sqrt{\frac{\hbar}{2M \omega}} = \sqrt{\frac{\hbar}{2M \sqrt{\frac{2k}{M}}}} = \left( \frac{\hbar^2}{2kM} \right)^{1/4}$$

Therefore, the allowed transitions are between those states for which (the selection rules)

$$\Delta m = \Delta n = 0, \Delta \ell = \pm 1$$

(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 $t$. 

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Between the states corresponding to energies $E_0$ and $E_1$, the selection rules allow only the transition $\psi_{000} \rightarrow \psi_{100}$. The corresponding probability is

\[
P_{10} = \frac{1}{\hbar^2} \left| \int_0^t H'_{10} e^{i\omega t} dt \right|^2 = \frac{A^2 \alpha^2}{\hbar^2} \left| \int_0^t \cos \omega t e^{i\omega t} dt \right|^2
\]

where we have used

\[
H'_{10} = \langle 100 | H'(x, t) | 000 \rangle = A_0 \cos \omega t
\]

Now,

\[
\int_0^t \cos \omega t e^{i\omega t} dt = \frac{1}{2i} \left[ e^{i(\omega + \bar{\omega})t} - 1 - \frac{e^{i(\omega - \bar{\omega})t} - 1}{\omega + \bar{\omega}} + \frac{e^{i(\omega - \bar{\omega})t} - 1}{\omega - \bar{\omega}} \right]
\]

In the microscopic world, $\omega$ and $\bar{\omega}$ are usually very large. Thus, only for $\omega \approx \bar{\omega}$, will the above integral be large. Thus,

\[
P_{10} \approx \frac{A^2 \alpha^2}{\hbar^2} \sin^2 \left( \frac{(\omega - \bar{\omega})t}{2} \right)
\]

or when $t$ gets large enough

\[
\frac{\sin^2 \left( \frac{(\omega - \bar{\omega})t}{2} \right)}{(\omega - \bar{\omega})^2} \rightarrow 2\pi t \delta(\omega - \bar{\omega})
\]

so that

\[
P_{10} \approx \frac{2\pi A^2 \alpha^2 t}{\hbar^2} \delta(\omega - \bar{\omega})
\]

and the transition rate is

\[
\frac{P_{10}}{t} \approx \frac{2\pi A^2 \alpha^2}{\hbar^2} \delta(\omega - \bar{\omega})
\]

### 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

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

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

To 1st–order the $1s \rightarrow 2s$ transition is forbidden since the matrix element $\langle 200 | z | 100 \rangle = 0$ by parity considerations. Likewise, since $z \propto Y_{10}$, which is a spherical tensor of rank 1, the corresponding matrix elements say that only the
1s → 2p (Δℓ = +1) transition is allowed in first order and we must also have Δm = 0.

With the potential energy

\[ V = -e\varepsilon_0 ze^{-t/\tau} \]

t for t > 0, we have the only non-vanishing first-order transition amplitude

\[ c^{(1)}(t) = -\left( -\frac{i}{\hbar} \right) e\varepsilon_0 \int_0^t dt \langle 210 | z | 100 \rangle e^{(i\omega - 1/\tau)t} \]

\[ = \frac{ie\varepsilon_0}{\hbar} \langle 210 | z | 100 \rangle \left( e^{(i\omega - 1/\tau)t} - 1 \right) \left( -i\omega - 1/\tau \right) \]

The probability is then

\[ P = \left| c^{(1)}(t) \right|^2 = \left( \frac{e\varepsilon_0}{\hbar} \right)^2 \frac{1}{\omega^2 + \frac{1}{\tau^2}} |\langle 210 | z | 100 \rangle|^2 \left( 1 + e^{-2t/\tau} - 2e^{-t/\tau} \cos \omega t \right) \]

For \( t \gg \tau \) (\( t \to \infty \) essentially) we have

\[ P = \left( \frac{e\varepsilon_0}{\hbar} \right)^2 \frac{1}{\omega^2 + \frac{1}{\tau^2}} |\langle 210 | z | 100 \rangle|^2 \]

Now,

\[ \langle 210 | z | 100 \rangle = 2\pi \int_{-1}^1 d(\cos \theta) \int_0^\infty r^2 dr R_{21} Y_{100 r} \cos \theta R_{10 Y00} = \frac{2^{15/2}}{3^3} a_0 \]

Therefore,

\[ P = \left( \frac{e\varepsilon_0}{\hbar} \right)^2 \frac{a_0^2}{\omega^2 + \frac{1}{\tau^2}} \frac{2^{15}}{3^{10}} \]

where

\[ \omega = \frac{E_{2p} - E_{1s}}{\hbar} = \frac{3e^2}{8a_0 \hbar} \]

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

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

Suppose the system is in the state \( |+\rangle |+\rangle \) 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.

We have (using the \(|S, S_z\rangle\) basis)

\[
\hat{H} = \left(\frac{4\Delta}{\hbar^2}\right) \hat{S}_1 \cdot \hat{S}_2 = 4\Delta \left(\frac{S^2 - S^2_1 - S^2_2}{2\hbar^2}\right) \to 4\Delta \left(\frac{S(S+1) - 3/2}{2}\right) = \begin{cases} 
\Delta & S = 1 \\
-3\Delta & S = 0 
\end{cases}
\]

so that

\[
\hat{H} |1, M\rangle = \Delta |1, M\rangle, \quad \hat{H} |0, 0\rangle = -3\Delta |0, 0\rangle
\]

We get the exact solution as follows: At \(t = 0\),

\[
|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|1, 0\rangle + |0, 0\rangle)
\]

At later \(t\),

\[
|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\Delta t/\hbar} |1, 0\rangle + e^{-i3\Delta t/\hbar} |0, 0\rangle\right)
\]

\[
= \frac{1}{2} \left(e^{-i\Delta t/\hbar} (|+\rangle + |-\rangle) + e^{-i3\Delta t/\hbar} (|+\rangle - |-\rangle)\right)
\]

\[
= \frac{1}{2} \left(\left(e^{-i\Delta t/\hbar} + e^{-i3\Delta t/\hbar}\right) |+\rangle + \left(e^{-i\Delta t/\hbar} - e^{-i3\Delta t/\hbar}\right) |-\rangle\right)
\]

Therefore,

\[
P_{+-}(t) = \langle + | \psi(t) \rangle^2 = \frac{1}{4} \left|e^{-i\Delta t/\hbar} + e^{-i3\Delta t/\hbar}\right|^2 = \frac{1}{2} + \frac{1}{2} \cos \frac{4\Delta t}{\hbar}
\]

\[
P_{-+}(t) = \langle - | \psi(t) \rangle^2 = \frac{1}{4} \left|e^{-i\Delta t/\hbar} - e^{-i3\Delta t/\hbar}\right|^2 = \frac{1}{2} - \frac{1}{2} \cos \frac{4\Delta t}{\hbar}
\]

\[
P_{++}(t) = \langle + | \psi(t) \rangle^2 = 0 = \langle - | \psi(t) \rangle^2 = P_{--}(t)
\]

(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?

Using first-order perturbation theory, we have

\[
c^{(1)}_{+\pi} = -\frac{i}{\hbar} \int_0^t (+ | \hat{H} | +\rangle) dt, \quad c^{(1)}_{-\pi} = -\frac{i}{\hbar} \int_0^t (- | \hat{H} | +\rangle) dt
\]

Now using,

\[
|+-\rangle = \frac{1}{\sqrt{2}} (|1, 0\rangle + |0, 0\rangle), \quad |-+\rangle = \frac{1}{\sqrt{2}} (|1, 0\rangle - |0, 0\rangle)
\]

we have

\[
c^{(1)}_{+\pi} = -\frac{i\Delta t}{\hbar} \left(\frac{1 - 3}{2}\right) = \frac{i\Delta t}{\hbar}, \quad c^{(1)}_{-\pi} = \frac{i\Delta t}{\hbar} \left(\frac{1 + 3}{2}\right) = -\frac{2i\Delta t}{\hbar}
\]
In addition, \( c_{++}^{(1)} = c_{--}^{(1)} = 0 \) because \( \hat{H} \) only connects states of the same 
\[ M_{\text{total}} = m_1 + m_2, \] 
which is zero for this initial state.

Therefore, we have

\[
\begin{align*}
P_{+-}(t) &= |c_{+-}(t)|^2 = \left| 1 + \frac{i\Delta t}{\hbar} \right|^2 = 1 + \frac{\Delta^2 t^2}{\hbar^2} \\
P_{-+}(t) &= |c_{-+}(t)|^2 = \left| -\frac{2i\Delta t}{\hbar} \right|^2 = \frac{4\Delta^2 t^2}{\hbar^2} \\
P_{++}(t) &= |c_{++}(t)|^2 = 0 = |c_{--}(t)|^2 = P_{--}(t)
\end{align*}
\]

We note that the exact solutions expanded to first order are

\[
\begin{align*}
P_{+-}(t) &= \frac{1}{2} - \frac{1}{2} \cos \frac{4\Delta t}{\hbar} = \frac{1}{2} - \frac{1}{2} \left( 1 - \frac{1}{2} \left( \frac{4\Delta t}{\hbar} \right)^2 \right) = \frac{4\Delta^2 t^2}{\hbar^2} \\
P_{-+}(t) &= \frac{1}{2} + \frac{1}{2} \cos \frac{4\Delta t}{\hbar} = \frac{1}{2} + \frac{1}{2} \left( 1 - \frac{1}{2} \left( \frac{4\Delta t}{\hbar} \right)^2 \right) = 1 - \frac{4\Delta^2 t^2}{\hbar^2}
\end{align*}
\]

in agreement with perturbation theory, but

\[
\begin{align*}
P_{+-}(t) &= \frac{1}{2} - \frac{1}{2} \cos \frac{4\Delta t}{\hbar} = \frac{1}{2} - \frac{1}{2} \left( 1 - \frac{1}{2} \left( \frac{4\Delta t}{\hbar} \right)^2 \right) = 1 - \frac{4\Delta^2 t^2}{\hbar^2}
\end{align*}
\]

which does not agree with perturbation theory.

We should not be surprised that something is wrong somewhere with the perturbation result since the total probability for something to happen is larger than one!

What is happening?

It turns out that there is another nonzero term to this order, in fact, the \( c_{+-}^{(2)} \) amplitude interferes with the \( c_{+-}^{(0)} \) amplitude and contributes \( \Delta^2 t^2 \) terms also.

If they are included, we get

\[
P_{+-}(t) = 1 - \frac{8\Delta^2 t^2}{\hbar^2}
\]

which is still not in agreement with the exact result.

It turns out that the validity of first-order perturbation theory for the \(|+-\rangle\) state is never satisfied.

The validity for the \(|-+\rangle\) state is questionable when \( t >> h/\Delta \) since the lowest order expression gives a poor approximation to the exact answer.

### 11.5.5 A Variational Calculation of the Deuteron Ground State Energy

Use the empirical potential energy function

\[
V(r) = -Ae^{-r/a}
\]

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where $A = 32.7 \text{MeV}$, $a = 2.18 \times 10^{-13} \text{cm}$, 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 $\alpha$ is the variational parameter to be determined. Calculate the energy in terms of $\alpha$ and minimize it. Give your results for $\alpha$ and $E$ in MeV. The experimental value of $E$ is $-2.23 \text{MeV}$ (your answer should be VERY close! Is your answer above this? [HINT: do not forget about the reduced mass in this problem])

We have

$$V(r) = -Ae^{-r/a}, \ A = 32.7 \text{MeV}, \ a = 2.18 \times 10^{-13} \text{cm}$$

We also assume that $\ell = 0$. Then

$$E_0 \leq \frac{\langle \psi|\hat{H}|\psi \rangle}{\langle \psi|\psi \rangle}$$

with

$$\hat{H} = -\frac{\hbar^2}{2m_D} \nabla^2 + V(r)$$

and we assume the trial function

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

We then have (using $\ell = 0$)

$$\nabla^2 \psi(r) = \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d \psi}{dr} \right) \frac{1}{r^2} \frac{d}{dr} \left( -\frac{\alpha}{2a} r^2 e^{-\alpha r/2a} \right)$$

$$= \frac{\alpha}{2a} \left( \frac{2}{r} - \frac{\alpha}{2a} \right) e^{-\alpha r/2a} = \left( -\frac{\alpha}{a} + \left( \frac{\alpha}{2a} \right)^2 \right) e^{-\alpha r/2a}$$

Therefore,

$$\langle \psi|\hat{H}|\psi \rangle = 4\pi \int_0^\infty r^2 dr e^{-\alpha r/a} \left( -\frac{\hbar^2}{2m_D} \left( -\frac{\alpha}{a} \frac{1}{r} + \left( \frac{\alpha}{2a} \right)^2 \right) - Ae^{-r/a} \right)$$

$$= 4\pi \left[ \frac{\hbar^2}{2m_D} \frac{\alpha}{a} \int_0^\infty r dr e^{-\alpha r/a} - \frac{\hbar^2}{2m_D} \left( \frac{\alpha}{2a} \right)^2 \int_0^\infty r^2 dr e^{-\alpha r/a} - A \int_0^\infty r^2 dr e^{-(1+\alpha)r/a} \right]$$

$$= 4\pi \left[ \frac{\hbar^2}{2m_D} \frac{\alpha}{a} \frac{1}{(\alpha/a)^2} - \frac{\hbar^2}{2m_D} \left( \frac{\alpha}{2a} \right)^2 \frac{2}{(\alpha/a)^3} - A \frac{2}{(1+\alpha)^3} \right]$$

$$= 4\pi \left[ \frac{\hbar^2}{4m_D} \frac{a}{\alpha} - 2A \frac{a^3}{(1+\alpha)^3} \right]$$

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and
\[
\langle \psi | \psi \rangle = 4\pi \int_0^\infty r^2 dr e^{-\alpha r/\alpha} = 4\pi \frac{2}{(\frac{a}{\alpha})^3} = 8\pi \left(\frac{a}{\alpha}\right)^3
\]
where we have used
\[
\int_0^\infty r^n e^{-\rho r} dr = \frac{n!}{\rho^{n+1}}
\]
Thus,
\[
E_0 \leq \frac{4\pi}{8\pi \left(\frac{a}{\alpha}\right)^3} \left[\frac{\alpha^2}{4m_D} - \frac{2A}{(1+\alpha)^2}\right] = \frac{1}{2} \alpha^2 \left(\frac{\hbar^2}{4m_D} - 2A\frac{a^2\alpha}{(1+\alpha)^3}\right)
\]
One solution is \(\alpha = 0 \rightarrow E_0 \leq 0\), which we already know is true; so we ignore this solution. The second solution is given by
\[
0 = \left(\frac{\hbar^2}{4m_D} - 2A\frac{a^2\alpha}{(1+\alpha)^3}\right) + \alpha \left(-A\frac{a^3}{(1+\alpha)^2} + 3A\frac{a^2\alpha}{(1+\alpha)^2}\right)
\]
\[
\frac{\hbar^2}{4m_D} (1+\alpha)^4 - 2Aa^2\alpha (1+\alpha) - Aa^3 (1+\alpha) + 3Aa^2\alpha^2 = 0
\]
\[
\frac{\hbar^2}{4m_D} (1+\alpha)^4 - 3Aa^2\alpha = 0
\]
\[(1+\alpha)^4 - \beta\alpha = 0 \quad , \quad \beta = \frac{12m_D Aa^2}{\hbar^2}
\]
Now
\[
A = 32.7 \text{ MeV} = 32.7 \times 10^6 \text{eV} \cdot 1.602 \times 10^{-19} J/\text{eV} = 5.239 \times 10^{-12} J
\]
\[
a^2 = (2.18 \times 10^{-13}) \text{cm}^2 \cdot 10^{-4} m^2/\text{cm}^2 = 4.752 \times 10^{-30} m^2
\]
\[
\hbar^2 = (1.054 \times 10^{-34})^2 J^2 - s^2 = 1.111 \times 10^{-68} J^2 - s^2
\]
\[
m_D = \frac{m_n m_p}{m_n + m_p} = \frac{1.672 \times 10^{-27} kg}{1.672 \times 10^{-27} kg} \times 10^{-27} kg = 0.835 \times 10^{-27} kg
\]
Therefore,
\[
\beta = \frac{12m_D Aa^2}{\hbar^2} = \frac{12 \cdot 0.835 \cdot 5.239 \cdot 4.752}{1.111} \times 10^{-1} = 22.453
\]
Therefore we must numerically solve the equation
\[(1+\alpha)^4 - 22.453\alpha = 0
\]
We find \(\alpha = 1.344\). Now
\[
\frac{\hbar^2}{4m_D a^2} = \frac{1.111}{4 \times 0.835 \times 4.752} \times 10^{-11} = 7.000 \times 10^{-13} J
\]
\[
\rightarrow \frac{1.111}{1.662 \times 10^{-13} J/\text{MeV} = 4.369 \text{MeV}}
\]
and
\[
E_0 \leq \frac{a^2}{2} \left(4.369 - 65.4 \frac{a}{(1+\alpha)^2}\right) = 2.185\alpha^2 - 32.7 \frac{\alpha^3}{(1+\alpha)^3}
\]
\[
E_0 \leq 2.185(1.344)^2 - 32.7 (\frac{1.344}{2.344})^3 = 3.947 - 6.164 = -2.217 \text{MeV}
\]
The experimentally measured value is \(-2.23 \text{MeV}\).
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.

For \( t < 0 \) and \( t > T \),

\[
\frac{1}{2}m\omega^2 x^2
\]

For \( 0 < t < T \),

\[
\frac{1}{2}m\omega^2 (x - a)^2 = \frac{1}{2}m\omega^2 x^2 - m\omega^2 ax + \frac{1}{2}m\omega^2 a^2
\]

For \( t < 0 \) and \( t > T \),

\[
H = H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \Rightarrow H_0 \varphi_n = \hbar \omega (n + 1/2) \varphi_n
\]

For \( 0 < t < T \),

\[
H = H_0 + W = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - m\omega^2 ax + \frac{1}{2}m\omega^2 a^2
\]

\[
W = -m\omega^2 ax + \frac{1}{2}m\omega^2 a^2
\]

Therefore,

\[
P_{fi} = \frac{1}{\hbar^2} \left| \int_0^T e^{i\omega_{fi}t'} W_{fi}(t') dt' \right|^2, \quad \omega_{fi} = \frac{1}{\hbar}(E_f - E_i)
\]

Now,

\[
W_{01} = -m\omega^2 a \langle \varphi_0 | x | \varphi_1 \rangle + \frac{1}{2}m\omega^2 a^2 \langle \varphi_0 | \varphi_1 \rangle
\]

\[
= -m\omega^2 a \sqrt{\frac{\hbar}{2m\omega}} \langle \varphi_0 | (a + a^+) | \varphi_1 \rangle = -m\omega^2 a \sqrt{\frac{\hbar}{2m\omega}}
\]

so that

\[
P_{01} = \frac{1}{\hbar^2} \left( -m\omega^2 a \sqrt{\frac{\hbar}{2m\omega}} \right)^2 \left| \int_0^T e^{i\omega_{fi}t'} dt' \right|^2 = \frac{2m\omega a^2}{\hbar} \sin^2 \left( \frac{\omega T}{2} \right)
\]

Also,

\[
W_{21} = -m\omega^2 a \langle \varphi_2 | x | \varphi_1 \rangle + \frac{1}{2}m\omega^2 a^2 \langle \varphi_2 | \varphi_1 \rangle
\]

\[
= -m\omega^2 a \sqrt{\frac{\hbar}{2m\omega}} \langle \varphi_2 | (a + a^+) | \varphi_1 \rangle = -m\omega^2 a \sqrt{\frac{\hbar}{m\omega}}
\]
so that

\[ P_{21} = \frac{1}{\hbar^2} \left( -m\omega^2 a \sqrt{\frac{\hbar}{m\omega}} \right)^2 \left| \int_0^T \int_0^{\omega_t} e^{i\omega_t \tau'} d\tau' \right|^2 = \frac{4 m \omega a^2}{\hbar} \sin^2 \left( \frac{\omega T}{2} \right) \]

In first-order perturbation theory, \( P_{n1} (n > 2) = 0 \) since \( \langle \varphi_n | W | \varphi_1 \rangle = 0 \) for \( n > 2 \).

### 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.

The Hamiltonian is

\[ \hat{H} = \frac{p^2}{2m} + \frac{1}{2} (2k)x^2 \]

(a) What are the energy eigenvalues of the particle when it is connected to both springs?

The energy eigenvalues are

\[ E_n = \hbar \bar{\omega}(n + 1/2) , \quad \bar{\omega} = \sqrt{\frac{2k}{m}} \]

(b) What is the wave function in the ground state?

The ground-state wave function is

\[ \langle x | \bar{0} \rangle = \psi_{\bar{0}}(x) = \left( \frac{m \bar{\omega}}{\pi \hbar} \right)^{1/4} e^{-\frac{m \bar{\omega} x^2}{2k}} \]

(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?

The new ground-state is that of a mass connected to one spring

\[ \langle x | 0 \rangle = \psi_0(x) = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} e^{-\frac{m \omega x^2}{2k}} , \quad \omega = \sqrt{\frac{k}{m}} \]

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In this sudden approximation, we have

\[ P(\text{remains in } |\bar{0}\rangle) = |\langle \bar{0} | 0 \rangle|^2 = \left| \int_{-\infty}^{\infty} \psi_0(x) \psi_{\bar{0}}(x) \, dx \right|^2 \]

\[ = \left| \int_{-\infty}^{\infty} \left( \frac{m \bar{\omega}}{\pi \hbar} \right)^{1/4} e^{-\frac{m \bar{\omega} x^2}{2 \hbar}} \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} e^{-\frac{m \omega x^2}{2 \hbar}} \, dx \right|^2 \]

\[ = \left( \frac{m \sqrt{2k}}{\pi \hbar} \right)^{1/2} \left( \frac{m \sqrt{k}}{\pi \hbar} \right)^{1/2} \left| \int_{-\infty}^{\infty} e^{-\frac{m \bar{\omega} x^2}{2 \hbar}} \, dx \right|^2 \]

\[ = 2^{1/4} \frac{m \sqrt{2k}}{\pi \hbar} \frac{2\hbar}{m(\sqrt{2} + 1) \sqrt{k}} \left| \int_{-\infty}^{\infty} e^{-y^2} \, dy \right|^2 \]

\[ = \frac{2^{1/4}}{\pi} \frac{2}{(1 + \sqrt{2}) \pi} = 0.985 \]

so the probability of remaining in the ground state is close to one.

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

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

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.

The initial state is \(|0\rangle\). The transition amplitudes are

\[ c_n^{(0)}(t) = \delta_{n0} \quad , \quad c_n^{(1)}(t) = -i \int_0^t e^{-i(E_0 - E_n)\frac{t}{\hbar}} \langle n | H'(x, t) | 0 \rangle \, dt \]

Now,

\[ \langle n | H'(x, t) | 0 \rangle = Ae^{-t/\tau} \langle n | x^2 | 0 \rangle = Ae^{-t/\tau} \frac{\hbar}{2m\omega} \langle n | (a + a^+)^2(a + a^+) | 0 \rangle \]

\[ = Ae^{-t/\tau} \frac{\hbar}{2m\omega} \langle n | (0) + \sqrt{2} | 2 \rangle = Ae^{-t/\tau} \frac{\hbar}{2m\omega} \left( \delta_{n0} + \sqrt{2}\delta_{n2} \right) \]

Therefore, \(c_n^{(1)}(t) = 0\) unless \(n = 0, 2\). We therefore have that

\[ c_n^{(0)}(t) = 0 = c_n^{(0)}(t) \]
and
\[ c_0^{(1)}(t) = -\frac{i}{\hbar} A \frac{\hbar}{2m\omega} \int_0^t e^{-t/\tau} dt = \frac{iA\tau}{2m\omega} \left( e^{-t/\tau} - 1 \right) \]

For \( t/\tau \gg 1 \), we then have
\[ c_0^{(1)}(t) = -\frac{iA\tau}{2m\omega} \]

In the same way,
\[ c_2^{(1)}(t) = -\frac{iA\sqrt{2}}{2m\omega} \left( e^{-t/\tau} - 1 \right) \]

Thus, after a long time duration of the perturbation, the state becomes
\[ |\psi\rangle = \left[ 1 - \frac{iA\tau}{2m\omega} e^{-i\omega t/2} |0\rangle - \frac{iA\sqrt{2}}{2m\omega (\frac{1}{\tau} - 2\omega i)} e^{-i5\omega t/2} |2\rangle \right] \]

(all higher order terms in \( A \), that is, \( A^2, A^3 < \ldots \) terms) are ignored).

Thus, the probability for the system to make a transition to the 2\textsuperscript{nd} excited state is
\[ P_2 = \left| \frac{A^2}{2m^2\omega^2 \left( \frac{1}{\tau^2} + 4\omega^2 \right)} \right|^2 \]
\[ \approx \frac{A^2}{2m^2\omega^2 \left( \frac{1}{\tau^2} + 4\omega^2 \right)} \]

There is no probability for a transition to \(|1\rangle\) or \(|3\rangle\).

### 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 \( \varphi_i(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_Z) \) and \( \varphi_f(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_Z) \), 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.

The initial state is
\[
\varphi_0 = \psi_{n\ell m}(\vec{r}) \varphi_i(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z)
\]
and the final state is
\[
\varphi_1 = \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{r}} \varphi_f(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z)
\]
where the final state is a plane wave, which is normalized in a box of volume \(V = L^3\) and we use periodic boundary conditions.

The matrix element needed to calculate the internal conversion rate is
\[
W_{01} = \langle \varphi_1 | W | \varphi_0 \rangle = -\frac{1}{\sqrt{V}} \int d^3r e^{-i\vec{k} \cdot \vec{r}} \langle \varphi_f(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z) | \sum_{j=1}^{Z} \frac{e^2}{|\vec{r} - \vec{r}_j|} | \varphi_i(\vec{r}_i, \vec{r}_2, ..., \vec{r}_Z) \rangle \psi_{n\ell m}(\vec{r})
\]

(b) Write down an expression for the internal conversion rate.

We find the internal conversion rate using Fermi’s golden rule
\[
W_{0 \rightarrow 1} = \frac{2\pi}{\hbar} \rho(E_1) |W_{01}|^2 \delta(E_1 - E_0)
\]
so that we need to find \(\rho(E_1)\).

The energy eigenstates of a free electron confined to a cubical box with periodic boundary conditions are
\[
\varphi_{n_x, n_y, n_z}(x, y, z) = \frac{1}{\sqrt{L^3}} e^{i\frac{2\pi}{L}(n_x x + n_y y + n_z z)}
\]
with \(n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots\). We have
\[
k_x = \frac{2\pi}{L} n_x, k_y = \frac{2\pi}{L} n_y, k_z = \frac{2\pi}{L} n_z
\]
If \(k\) is large, then the number of states with a wave vector whose magnitude lies between \(k\) and \(k + dk\) is
\[
dN = \frac{4\pi k^2 dk}{(2\pi)^3} = \frac{\text{volume of shell}}{\text{volume per state}}
\]
so that
\[
\frac{dN}{dk} = \frac{4\pi V k^2}{(2\pi)^3}
\]
The density of states is
\[
\frac{dN}{dE} = \frac{dN}{dk} \frac{dk}{dE}
\]

Using
\[
E = \frac{\hbar^2 k^2}{2m}
\]
we find
\[
\frac{dN}{dE} = \frac{mvk}{2\pi^2 \hbar^2} = \frac{(2m)^{3/2} V}{4\pi^2 \hbar^3} \sqrt{E}
\]
(if we do not neglect spin, we would multiply by 2).

We therefore have for the internal conversion rate
\[
W_{0 \rightarrow 1} = \frac{2\pi}{r} \left( \frac{2m}{\pi \hbar^2} \right)^{3/2} \sqrt{E_1}
\times \left| \int d^3r e^{-i\vec{k} \cdot \vec{r}} \langle \phi_f(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z) | \sum_{j=1}^Z \frac{e^2}{|\vec{r} - \vec{r}_j|} | \phi_i(\vec{r}_i, \vec{r}_2, ..., \vec{r}_Z) \rangle \psi_{n\ell m}(\vec{r}) \right|^2 \delta(E_1 - E_0)
\]
(c) For light nuclei, the nuclear radius is much smaller than the Bohr radius for a given \(Z\), 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
\[
\vec{d} = \langle \phi_f \sum_{j=1}^Z \frac{e^2}{|\vec{r} - \vec{r}_j|} | \phi_i \rangle
\]
Using
\[
\frac{1}{|\vec{r} - \vec{r}_j|} \approx \frac{1}{r} \frac{\vec{r} \cdot \vec{r}_j}{r^3}
\]
we have
\[
\langle \phi_f(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z) | \sum_{j=1}^Z \frac{e^2}{|\vec{r} - \vec{r}_j|} | \phi_i(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z) \rangle = \frac{e^2}{r^3} \vec{r} \cdot \vec{d}
\]
where \(\vec{d}\) is independent of \(\vec{r}\). We can therefore write
\[
W_{0 \rightarrow 1} = \frac{e^4}{2\pi \hbar} \left( \frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E_1} \left| \int d^3r e^{-i\vec{k} \cdot \vec{r}} \frac{e^2}{r^3} \psi_{n\ell m}(\vec{r}) \right|^2 \delta(E_1 - E_0)
\]
Note that in the above result we have used
\[
\frac{e^2}{r} \langle \phi_f(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z) | \hat{I} | \phi_i(\vec{r}_1, \vec{r}_2, ..., \vec{r}_Z) \rangle = 0
\]
11.5.10 Time Evolution Operator

A one-dimensional anharmonic oscillator is given by the Hamiltonian

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

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

Using

$$O_I(t) = e^{iH_0 t/\hbar} O e^{-iH_0 t/\hbar}$$

and

$$[a, a^\dagger] = 1$$

we get

$$\frac{\partial a^\dagger}{\partial t} = \frac{i}{\hbar}[H_0, a^\dagger] = \frac{i}{\hbar} e^{iH_0 t/\hbar} [H_0, a^\dagger] e^{-iH_0 t/\hbar}$$

$$= i\omega e^{iH_0 t/\hbar}[a^\dagger a, a^\dagger] e^{-iH_0 t/\hbar} = i\omega e^{iH_0 t/\hbar}(a^\dagger aa^\dagger - a^\dagger a^\dagger a)e^{-iH_0 t/\hbar}$$

$$= i\omega e^{iH_0 t/\hbar} a^\dagger [a, a^\dagger] e^{-iH_0 t/\hbar} = i\omega a^\dagger$$

which implies that

$$a^\dagger_I = e^{i\omega t} a^\dagger$$

which fulfills the condition $a^\dagger_I(t = 0) = a^\dagger$. We then have $a_I = e^{-i\omega t} a$

The perturbation in the interaction representation is then

$$V_I = \lambda a^\dagger a_I a_I = \lambda a^\dagger aae^{-i\omega t}$$

The time evolution operator is now obtained to lowest order from

$$U(t, t_0) \approx I - \frac{i}{\hbar} \int_{t_0}^t dt' V_I = I - \frac{i\lambda}{\hbar} a^\dagger a e^{-i\omega t} = I - \frac{\lambda}{\hbar \omega} a^\dagger a e^{-i\omega t}$$

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 $H'(t) = U\delta(t)$ where the operator $U$ has only off-diagonal matrix elements (call them $U$). If the system is initially in the state $a$, find the probability $P_{a\rightarrow b}$ that a transition occurs. Use only the lowest order of perturbation theory that gives a nonzero result.

We have

$$d_b = \frac{i}{\hbar} \int_0^t \langle \psi_b | H'(t') | \psi_a \rangle e^{i\omega_{ba} t'} dt'$$

$$= -\frac{i}{\hbar} \int_0^t \langle \psi_b | U\delta(t') | \psi_a \rangle e^{i\omega_{ba} t'} dt' = -\frac{i}{\hbar} \langle \psi_b | U | \psi_a \rangle$$
Then,

\[ \text{Prob}(a \rightarrow b) = |d_b|^2 = \frac{U^2}{\hbar^2} \]

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?

We have

\[ H_{\text{old}} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \rightarrow \hbar \omega (a^+ a + 1/2) \rightarrow |0\rangle_{\text{old}} = |0\rangle \]

and

\[ H_{\text{new}} = \frac{(p + p_0)^2}{2m} + \frac{1}{2}m\omega^2 x^2 = H_{\text{old}} + \frac{p_0 p}{m} + \frac{p_0^2}{2m} \]

or

\[ H_{\text{new}} = \hbar \omega (a^+ a + 1/2) + \frac{p_0}{m} \sqrt{\frac{m \hbar \omega}{2}} (a - a^+) + \frac{p_0^2}{2m} \]

Now define \( a = A + \beta \). This says that

\[ [a, a^+] = 1 = [A, A^+] \]

and if we choose

\[ \beta = \frac{i p_0}{m} \sqrt{\frac{m \hbar \omega}{2}} \]

\[ H_{\text{new}} = \hbar \omega (A^+ A + 1/2) + \frac{\hbar \omega}{4} \]

which is another harmonic oscillator with shifted energies.

The new ground state is defined by

\[ A |0\rangle_{\text{new}} = 0 = (a - \beta) |0\rangle_{\text{new}} \]

or

\[ a |0\rangle_{\text{new}} = \beta |0\rangle_{\text{new}} \]

Thus, \( |0\rangle_{\text{new}} \) is a coherent state, i.e.,

\[ |0\rangle_{\text{new}} = |\beta\rangle \]

where

\[ a |\beta\rangle = \beta |\beta\rangle \]

Thus,

\[ |0\rangle_{\text{new}} = e^{\beta^2/2} \sum_{m=0}^{\infty} \frac{\beta^m}{\sqrt{m!}} |m\rangle \]
Therefore,

\[ \langle 0 | 0 \rangle_{new} = e^{\beta^2/2} \]

and the probability of remaining in the old ground state is

\[ \text{Prob} = |\langle 0 | 0 \rangle_{new}|^2 = e^{\beta^2} = e^{-p_0^2/2m\hbar\omega} \]

11.5.13 Hydrogen beam between parallel plates

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

![Figure 11.1: Hydrogen beam between parallel plates](image)

All of the \( n = 2 \) states of hydrogen are degenerate in the absence of the field \( \vec{E} \), 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?

Consider the potential energy \( e\vec{E}z \) of the electron (charge = \( -e \)) of a hydrogen atom in the external electric field \( \vec{E} \) as a perturbation \( H' \). Since the \( n = 2 \) states are degenerate, we need to calculate matrix elements of the form \( \langle 2\ell'm' | H' | 2\ell'm \rangle \).

The selection rules for this perturbation imply that

\[ \Delta \ell = \pm 1 \quad , \quad \Delta m = 0 \]

Thus the perturbation matrix is

\[
\begin{pmatrix}
0 & \langle 200 | z | 210 \rangle & 0 & 0 \\
\langle 210 | z | 200 \rangle & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
= \begin{pmatrix}
0 & -3e\vec{E}a_0 & 0 & 0 \\
-3e\vec{E}a_0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]

that is, only the (200) and (210) states are connected (mixed) by the perturbation.
(b) Find the linear combination of the \( n = 2 \) states which removes the degeneracy as much as possible.

The eigenvalues and eigenvectors of the \( 2 \times 2 \) submatrix are

\[
E = 3e\mathcal{E}a_0 \rightarrow |+\rangle = \frac{1}{\sqrt{2}} (|200\rangle + |210\rangle), \quad E = -3e\mathcal{E}a_0 \rightarrow |-\rangle = \frac{1}{\sqrt{2}} (|200\rangle - |210\rangle)
\]

and thus the degeneracy is removed for these two states (it remains for the \((211)\) and \((21-1)\) states.

(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.

We have

\[
|\psi(0)\rangle = |2s\rangle = |200\rangle = \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle)
\]

At time \( 0 < t \leq L/v \) when the atoms are subject to the electric field,

\[
|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left( e^{i3e\mathcal{E}a_0 t/\hbar} |+\rangle + e^{-i3e\mathcal{E}a_0 t/\hbar} |-\rangle \right) = \begin{pmatrix} \cos (3e\mathcal{E}a_0 t/\hbar) \\ i \sin (3e\mathcal{E}a_0 t/\hbar) \end{pmatrix}
\]

\[
= \cos (3e\mathcal{E}a_0 t/\hbar) |2s\rangle + i \sin (3e\mathcal{E}a_0 t/\hbar) |2p\rangle
\]

(d) Find the probability that the emergent beam contains hydrogen in the various \( n = 2 \) states.

This says that for \( t > L/v \) we have the probabilities

\[
|\langle 200 | \psi(t) \rangle|^2 = |\langle 2s | \psi(t) \rangle|^2 = \cos^2 (3e\mathcal{E}a_0 t/\hbar)
\]

\[
|\langle 210 | \psi(t) \rangle|^2 = |\langle 2p | \psi(t) \rangle|^2 = \sin^2 (3e\mathcal{E}a_0 t/\hbar)
\]

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](image)

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 \( V(x) = -A\delta(x) \).

The energy eigenfunction \( \psi \) satisfies the Schrödinger equation

\[
-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - A\delta(x)\psi = E\psi, \quad E < 0
\]

or

\[
\frac{d^2\psi}{dx^2} - k^2\psi + A_0\delta(x)\psi = 0, \quad |E| = \frac{\hbar^2 k^2}{2m}, \quad A_0 = \frac{2mA}{\hbar^2}
\]

Integrating from \(-\varepsilon \rightarrow +\varepsilon\), \( \varepsilon \) being an arbitrarily small, positive number and then letting \( \varepsilon \rightarrow 0 \), we get

\[
\psi'(0^+) - \psi'(0^-) = -A_0\psi(0)
\]

We also have wave function continuity at \( x = 0 \)

\[
\psi(0+) = \psi(0-) = \psi(0)
\]

Therefore,

\[
\frac{\psi'(0^+)}{\psi(0^+)} - \frac{\psi'(0^-)}{\psi(0^-)} = -A_0
\]

Now, for \( x \neq 0 \), the Schrödinger equation has the solution

\[
\psi(x) = Ce^{-k|x|}
\]

so that

\[
\psi(x) = Ce^{-kx}, \quad x > 0, \quad \psi(x) = Ce^{kx}, \quad x < 0
\]

and thus

\[
\frac{\psi'(0^+)}{\psi(0^+)} = -2k \rightarrow k = \frac{A_0}{2} = \frac{mA}{\hbar^2}
\]

The energy level for the bound state is

\[
E = -\frac{\hbar^2 k^2}{2m} = -\frac{mA^2}{2\hbar^2}
\]

and the corresponding normalized eigenfunction is

\[
\psi(x) = \sqrt{\frac{mA}{\hbar^2}} e^{-\frac{mA}{\hbar^2} |x|}
\]

(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 \( E_k \), \( D(E_k) \).
If the unbound states can be approximated by a plane wave $e^{ikx}$ in a 1-dimensional box of length $L$ with periodic boundary conditions, we have

$$e^{ikL/2} = e^{-ikL/2} \rightarrow e^{ikL} = 1 \rightarrow kL = 2n\pi \ , \ n = 0, \pm 1, \pm 2, \ldots.$$ 

so that

$$k_n = \frac{2n\pi}{L}$$

The normalized plane wave function for the wave vector $k$ is

$$\psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx} = \frac{1}{\sqrt{L}} e^{i\frac{2n\pi x}{L}}$$

Note that the state of energy $E_k$ is 2-fold degenerate when $k \neq 0$ so that the number of state with momentum between $p$ and $p + dp$ is

$$\frac{Ldp}{2\pi\hbar} = \# \text{ cells in phase space} = D(k)dk = \frac{1}{2}D(E_k)dE_k$$

Now,

$$E_k = \frac{\hbar^2k^2}{2m} \rightarrow dE_k = \frac{\hbar^2k}{m} dk \ , \ k = \frac{p}{\hbar} \rightarrow E_k = \frac{p^2}{2m}$$

or

$$\frac{Ldp}{2\pi\hbar} = D(k)dk \rightarrow D(k) = \frac{L}{2\pi} \ , \ D(k)dk = \frac{1}{2}D(E_k) \frac{\hbar^2k}{m} dk$$

$$D(E_k) = \frac{L}{2\pi} \frac{m}{k^2} = \frac{L}{2\pi} \frac{m}{p} = \frac{L}{2\pi} \frac{m}{\sqrt{2mE_k}} = \frac{L}{2\pi} \sqrt{\frac{m}{2E_k}}$$

(c) Assume that the electric field may be treated as a perturbation. Write down the perturbation term in the Hamiltonian, $H_1$, and find the matrix element of $H_1$ between the initial and the final state $\langle 0 | H_1 | k \rangle$.

Treating the electric field effect as a perturbation we have

$$H' = -q\mathcal{E}_0 x$$

Its matrix element between the initial and final states is

$$\langle k | H' | 0 \rangle = \int_{-\infty}^{\infty} \psi_k^*(-q\mathcal{E}_0 x)\psi dx = -\frac{q\mathcal{E}_0}{\sqrt{L}} \sqrt{\frac{m\mathcal{A}}{\hbar^2}} \int_{-\infty}^{\infty} xe^{-ikx-k_0|x|} dx$$

or

$$\langle k | H' | 0 \rangle = \int_{-\infty}^{\infty} \psi_k^*(-q\mathcal{E}_0 x)\psi dx = -\frac{q\mathcal{E}_0}{\sqrt{L}} \sqrt{\frac{m\mathcal{A}}{\hbar^2}} \int_{-\infty}^{\infty} xe^{-ikx-k_0|x|} dx$$

$$= \frac{q\mathcal{E}_0}{\sqrt{L}} \sqrt{\frac{m\mathcal{A}}{\hbar^2}} \frac{d}{dk} \int_{-\infty}^{\infty} e^{-ikx-k_0|x|} dx$$

$$= \frac{q\mathcal{E}_0}{\sqrt{L}} \sqrt{\frac{m\mathcal{A}}{\hbar^2}} \left( -4i\mathcal{E}_0 \right) \frac{1}{(k^2 + k_0^2)^2}$$

$$= 4iq\mathcal{E}_0 \left( \frac{m\mathcal{A}}{\hbar^2} \right)^{3/2} \frac{k}{(k^2 + (\frac{m\mathcal{A}}{\hbar^2})^2)}$$

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(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

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

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 $t > \tau$.

The perturbation is

$$\hat{H}_1 = \begin{cases} 0 & -\infty < t < 0 \\ -qE_0 x & 0 \leq t \leq \tau \\ 0 & t > \tau \end{cases}$$

The transition probability at $t > \tau$ is

$$\varphi_{I\rightarrow F}(t) = \frac{1}{\hbar^2} \left| \langle k | \hat{H}_1 | 0 \rangle \right|^2 \left| \int_{0}^{\tau} e^{i\omega_{FI} t'} dt' \right|^2 = \frac{1}{\hbar^2} \left| \langle k | \hat{H}_1 | 0 \rangle \right|^2 \frac{\sin^2 (\omega_{FI} \tau/2)}{(\omega_{FI}/2)^2}$$

Since

$$E_F = \frac{\hbar^2 k^2}{2m} \quad , \quad E_I = -\frac{m A^2}{2\hbar^2} \quad , \quad \omega_{FI} = \frac{1}{\hbar} (E_F - E_I)$$

we get

$$\frac{\sin^2 (\omega_{FI} \tau/2)}{(\omega_{FI}/2)^2} = \frac{\sin^2 \left( \frac{\hbar \tau}{4m} \left( \frac{k^2}{\hbar^2} + \left( \frac{m A}{\hbar^2} \right)^2 \right) \right)}{\left( \frac{\hbar}{4m} \left( \frac{k^2}{\hbar^2} + \left( \frac{m A}{\hbar^2} \right)^2 \right) \right)^2}$$

and the probability is given by

$$P(E_k) dE_k = \varphi_{I\rightarrow F}(t) D(E_k) dE_k = \frac{1}{\hbar^2} \left| \langle k | \hat{H}_1 | 0 \rangle \right|^2 \frac{\sin^2 (\omega_{FI} \tau/2)}{(\omega_{FI}/2)^2} \frac{L}{\pi \hbar} \sqrt{\frac{m}{2E_k}} dE_k$$

$$= \frac{1}{\hbar^2} \left| \frac{4i q E_0}{\sqrt{L}} \left( \frac{m A}{\hbar^2} \right)^{3/2} \frac{k}{\left( \frac{k^2}{\hbar^2} + \left( \frac{m A}{\hbar^2} \right)^2 \right)^2} \right|^2 \frac{\sin^2 (\omega_{FI} \tau/2)}{(\omega_{FI}/2)^2} \frac{L}{\pi \hbar} \sqrt{\frac{m}{2E_k}} dE_k$$

$$= \frac{1}{\hbar^2} \left| \frac{4i q E_0}{\sqrt{L}} \left( \frac{m A}{\hbar^2} \right)^{3/2} \frac{k}{\left( \frac{k^2}{\hbar^2} + \left( \frac{m A}{\hbar^2} \right)^2 \right)^2} \right|^2 \frac{\sin^2 \left( \frac{h \tau}{4m} \left( \frac{k^2}{\hbar^2} + \left( \frac{m A}{\hbar^2} \right)^2 \right) \right)}{\left( \frac{h}{4m} \left( \frac{k^2}{\hbar^2} + \left( \frac{m A}{\hbar^2} \right)^2 \right) \right)^2} \frac{L}{\pi \hbar} \sqrt{\frac{m}{2E_k}} dE_k$$

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

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

At $t = -\infty$, the oscillator is known to be in the ground state. Using time-dependent perturbation theory to 1st-order, calculate the probability that the oscillator is found in the 1st 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 $\tau$; yet for $\tau >> 1/\omega$, the probability for excitation is essentially negligible. Is this reasonable?

We have a perturbation potential

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

The ground state energy is

$$E_0 = \frac{1}{2} \hbar \omega$$

and the first excited state energy is

$$E_1 = \frac{3}{2} \hbar \omega$$

so that

$$\omega_{10} = \frac{1}{\hbar}(E_1 - E_0) = \frac{\omega}{2}$$

We then have

$$e_1^{(1)} (\infty) = \frac{i}{\hbar} \frac{F_0 \tau}{\omega} \langle 1 | x | 0 \rangle \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\tau^2 + t^2} dt$$

Now we do the integral using the residue theorem. We choose the contour

real axis $[-R, R]$ + semicircle of radius $R$ closed in upper half-plane

This contour encloses a pole of the integrand at $+i\tau$. We have

$$\lim_{R \to \infty} \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{(z + i\tau)(z - i\tau)} dz = \frac{2\pi i}{\pi(\tau^2 + \tau^2)} = 2\pi i \text{Residue}(z = i\tau)$$

$$\int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\tau^2 + t^2} dt = \frac{2\pi i}{\pi} \frac{e^{-\omega \tau}}{2i\tau} = \frac{\pi e^{-\omega \tau}}{\tau}$$
We also have
\[ |1\rangle x 0 = \sqrt{\frac{\hbar}{2m\omega}} \]
so that
\[ c_1^{(1)}(\infty) = \frac{i}{\hbar} \frac{F_0\tau}{\omega} \sqrt{\frac{\hbar}{2m\omega}} \frac{\pi e^{-\omega\tau}}{\tau} \]
Therefore, the probability of the system being found in the first excited state is
\[ P_1 = |c_1^{(1)}(\infty)|^2 = \frac{\pi^2 F_0^2}{2m\hbar\omega^3} e^{-2\omega\tau} \]

**Challenge:** It is reasonable! If the perturbation is turned on very slowly, and then turned off very slowly (as in the \( \tau \gg 1/\omega \) case), then the oscillator can be visualized to be in the ground state all the time. This is so because the only effect of the applied force (uniform in space) is just a slow change in the equilibrium point of the oscillator. At each instant of time, we can solve the time-independent Schrödinger equation for the ground state.

### 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,

\[ \Gamma = \frac{4}{3\hbar} k^3 \sum_g |\langle \psi_g \mid \hat{d} \mid \psi_e \rangle|^2 \]

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

\[ \Gamma_{(nLJM_J) \rightarrow (n'LM_J')} = \frac{4}{3\hbar} k^3 \sum_{M_J'} |\langle n'LM_J' \mid \hat{d} \mid nLJM_J \rangle|^2 \]

The spontaneous decay rate on a dipole transition \( |\psi_e\rangle \rightarrow |\psi_g\rangle \) summed over all possible final states is (Fermi Golden Rule)

\[ \Gamma = \frac{4}{3\hbar} k^3 \sum_g |\langle \psi_g \mid \hat{d} \mid \psi_e \rangle|^2 \]

Including the Hydrogen fine-structure

\( (nLJM_J) \rightarrow \sum_{M_J'} (n'LJM_J') \)
we have
\[ \Gamma = \frac{4}{3\hbar} k^3 \sum_{M'_{J}} |\langle n' L' J' M'_{J} | \hat{d} | n L J M_{J} \rangle |^2 \]

(a) Show that the spontaneous emission rate is independent of the initial \( M_{J} \).
Explain this result physically.

Expand in the spherical basis
\[ \hat{d} = \sum_{q} e^{*}_{q \hat{d}_{q}} \]
and use the Wigner-Eckhart theorem
\[ \Gamma = \frac{4}{3\hbar} k^3 |\langle n' L' J' || d || n L J \rangle|^2 \sum_{q,M_{J}} |\langle J' M'_{J} | 1 q J M_{J} \rangle |^2 \]
But
\[ \sum_{q,M_{J}} |\langle J' M'_{J} | 1 q J M_{J} \rangle |^2 = 1 \]
by normalization. Therefore,
\[ \Gamma = \frac{4}{3\hbar} k^3 |\langle n' L' J' || d || n L J \rangle|^2 \]
independent of \( M_{J} \). This makes sense physically. The vacuum is isotropic
and will not care what direction the angular momentum is pointing in!

ASIDE: Note that \( \Gamma \propto \omega^3 \). Thus, high frequency transitions decay much
more rapidly than low frequency transitions. This makes sense from clas-
sical electromagnetic theory. The Larmor power (rate of energy from an
oscillating dipole) goes as \( \omega^3 \).

(b) Calculate the lifetime \( (\tau = 1/\Gamma) \) of the \( 2 P_{1/2} \) state in seconds.

We have the allowed transitions with associated CG coefficients

![Diagram of allowed transitions]

where we note that the Lamb shift puts \( 2 s_{1/2} \) above \( 2 p_{1/2} \). Also note the
branching ratios for the decay are \( 1/3 + 2/3 = 1 \).
From part (a), we need only consider one initial $M_J$ since $\Gamma$ is the same for all. Thus,
\[ \Gamma(2p_{1/2}) = \frac{4}{3\hbar} k^3 |\langle 2s_{1/2} | d | 2p_{1/2} \rangle|^2 \]
To calculate the reduced matrix element, pick some allowed transition and use the Wigner-Eckhart theorem.
\[ \langle 1s_{1/2}, M_J = 1/2 | \hat{d}_z | 2p_{1/2}, M_J = 1/2 \rangle = \langle 1s_{1/2} | d | 1/2, 1/2 | 101/21/2 \rangle \]
where $\langle 1/2, 1/2 | 101/21/2 \rangle = -1/\sqrt{3}$. We must now uncouple spin and orbital angular momentum in the LHS. We have
\[ |2p_{1/2}, 1/2\rangle = \sqrt{\frac{1}{3}} |2p, 0\rangle |1/2\rangle - \sqrt{\frac{2}{3}} |2p, 1\rangle |1/2\rangle \]
\[ |1s_{1/2}, 1/2\rangle = |1s, 0\rangle |1/2\rangle \]
This implies that
\[ \langle 1s_{1/2}, M_J = 1/2 | \hat{d}_z | 2p_{1/2}, M_J = 1/2 \rangle = \sqrt{\frac{1}{3}} \langle 1s, 0 | \hat{d}_z | 2p, 0 \rangle = -\frac{e}{\sqrt{3}} \langle 1s, 0 | \hat{z} | 2p, 0 \rangle \]
ASIDE: we have
\[ \langle 1s, 0 | \hat{z} | 2p, 0 \rangle = \int d^3x \psi_{2s,0}(\vec{x}) \hat{z} \psi_{2p,0}(\vec{x}) \]
and
\[ z = \sqrt{\frac{4\pi}{3}} Y_{10}(\theta, \phi) \]
Therefore,
\[ \langle 1s, 0 | \hat{z} | 2p, 0 \rangle = \sqrt{\frac{4\pi}{3}} \int_0^\infty dr u_{10} r u_{20} \int d\Omega Y_{00} Y_{10} Y_{10} \]
Now
\[ \int_0^\infty dr u_{10} r u_{20} = \frac{a_0}{\sqrt{6}} \int_0^\infty dq q^4 e^{-3q^2/2} = 1.29 a_0 \]
and
\[ \int d\Omega Y_{00} Y_{10} Y_{10} = \frac{1}{\sqrt{4\pi}} \int d\Omega Y_{10} Y_{10} = \frac{1}{\sqrt{4\pi}} \]
Therefore,
\[ \langle 1s_{1/2}, M_J = 1/2 | \hat{d}_z | 2p_{1/2}, M_J = 1/2 \rangle = -\frac{e}{\sqrt{3}} \sqrt{\frac{4\pi}{3}} (1.29 a_0) \frac{1}{\sqrt{4\pi}} = -0.43 e a_0 \]
Thus, we have
\[ \langle 1s_{1/2} | d | 2p_{1/2} \rangle = \sqrt{30} 0.43 e a_0 = 0.74 e a_0 \]
Thus,

\[ \Gamma(2p_{1/2}) = (0.74)^2 \frac{4}{3} \hbar^3 (\epsilon a_0)^2 \]

In atomic units:

\[ \frac{\hbar \Gamma}{e^2/a_0} = \frac{4}{3} (\epsilon a_0)^3 \left( \frac{\langle d \rangle}{\epsilon a_0} \right)^2 \]
\[ k = \frac{\omega}{c} = \frac{\hbar}{\epsilon c} = \epsilon \frac{e^2}{\epsilon \hbar c^2} = \alpha \frac{1}{\alpha_0} \]
\[ \rightarrow \frac{\hbar \Gamma}{e^2/a_0} = \epsilon^{3/4} \alpha^{3/2} (\epsilon a_0)^3 \]

Now,

\[ \frac{\langle d \rangle}{\epsilon a_0} = 0.74 \quad , \quad \alpha = \frac{1}{137} \]

and for \( n = 2 \rightarrow n = 1 \),

\[ \epsilon = \frac{\hbar \omega}{E_0} = \frac{3}{8} \]

Thus,

\[ \frac{\hbar \Gamma}{e^2/a_0} = 1.5 \times 10^{-8} \]

Since

\[ \frac{e^2}{a_0} = 27.2 \text{ eV} = 4.1 \times 10^{16} \text{ sec}^{-1} \]

we get \( \Gamma = 6.2 \times 10^8 \text{ sec}^{-1} \) and thus the lifetime is

\[ \tau = \frac{1}{\Gamma} = 1.6 \text{ ns} \]

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 \( \mathcal{E} = \mathcal{E} \hat{x} \) 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?

This problem is solved in Section 8.6.2 of the text. The new ground state is a coherent state of the old oscillator with \( a |\alpha \rangle = \alpha |\alpha \rangle \) where \( \alpha = e \mathcal{E} x_0 / \hbar \omega \), i.e.,

\[ |0\rangle_{\text{new}} = |\alpha \rangle = e^{-|\alpha|^2/2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} |m\rangle \]
where
\[ x_0 = \sqrt{\frac{\hbar}{2m\omega}} \]

The new ground state energy is the old ground state energy shifted by
\[ e^2 E^2 x_0^2 \frac{1}{\hbar \omega} \]
i.e.,
\[ E_{0, new} = E_{0, old} - \frac{e^2 E^2 x_0^2}{\hbar \omega} = \frac{\hbar \omega}{2} e^2 E^2 x_0^2 \]

(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?

In this case we can use the sudden approximation. We get
\[ Prob = |\langle 0 | 0 \rangle_{new}|^2 = e^{-|\alpha|^2} \]

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
\[ \hat{V}_1 = \frac{1}{2} k \langle - | \langle - | \otimes |\vec{r}|^2 \]

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

where $I^{CM}$ 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 $|\Psi_0\rangle$.

We will denote states in the Hilbert space by
\[ |\Psi\rangle = |s\rangle \otimes |\psi\rangle = |s; \psi\rangle \]

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The first thing to do is to examine the potential

\[ \hat{V}_1 = \frac{1}{2} k | - \rangle \langle - | \otimes | r \rangle \]

This potential corresponds to states of positive spin \(|+\rangle\) being in a free potential and states of negative spin \(|-\rangle\) being in a harmonic oscillator potential. The wave functions of the 3D harmonic oscillator can be obtained by separation of variables in Cartesian coordinates giving

\[ |n_x n_y n_z \rangle = |n_x \rangle \otimes |n_y \rangle \otimes |n_z \rangle \]

or

\[ \psi_{n_x n_y n_z}(\vec{x}) = \psi_{n_x}(x) \psi_{n_y}(y) \psi_{n_z}(z) \]

with energies

\[ E_{n_x n_y n_z} = \hbar \omega (n_x + n_y + n_z + 3/2) \quad n_x, n_y, n_z = 0, 1, 2, \ldots \]

Alternatively, you could obtain the wavefunction in spherical coordinates giving eigenfunctions

\[ \psi_{n\ell m}(\vec{x}) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \]

where

\[ R_{n\ell}(r) = r^\ell f_{n\ell}(r) e^{-\beta r^2} \]

with

\[ \beta = \frac{m \omega}{2 \hbar} \]

and

\[ f_{n\ell}(r) = \sum_k a_k r^k \]

defined by the recursion relation

\[ a_{k+2} = 2\beta \frac{2k - 4n}{(k+2)(k+2\ell+3)} a_k \quad k \geq 0, \text{ even} \]

\( a_0 \) is determined by the normalization and \( a_k = 0 \) for all other \( k \). The energies are

\[ E_{n\ell m} = \hbar \omega (2n + \ell + 3/2) \quad n, \ell = 0, 1, 2, \ldots \quad m = -\ell, -\ell + 1, \ldots, \ell - 1, \ell \]

It is interesting to note that this gives a better explanation for the energy level degeneracies of the 3D harmonic oscillator, i.e.,

\[ d(N) = \frac{(N+2)(N+1)}{2} \quad \text{for} \quad E_N = \hbar \omega (N + 3/2) \]

The reason for mentioning the spherical coordinate eigenfunctions was to specifically make clear that the ground state

\[ \langle \vec{x} | 0 \rangle = \psi_{n_x=0, n_y=0, n_z=0}(\vec{x}) = \psi_{n_x=0, \ell=0, m=0}(\vec{x}) = \left( \frac{m \omega}{2 \hbar} \right)^{3/4} e^{-\omega (x^2 + y^2 + z^2)/2\hbar} = \left( \frac{2\beta}{\pi} \right)^{3/4} e^{-\beta r^2} \]
is an $\ell = m = 0$ state (you could also deduce that from the fact that it has no angular dependence when written in spherical coordinates).

In order to better demonstrate how to find transition rates (and to double check my results) I will calculate the transition rate using two different options: transitions to plane waves and transitions to spherical waves. I will define the continuum states $|\vec{k}\rangle$ and $|k\rangle$ to be the plane wave and spherical $s$-wave (respectively) with delta function normalizations:

$$\langle \vec{x} | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k} \cdot \vec{x}}$$

$$\langle k | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} \int d^3 \vec{x} e^{i(\vec{k} - \vec{k}) \cdot \vec{x}} = \delta^3(\vec{k} - \vec{k}')$$

$$\langle \vec{x} | k \rangle = \frac{k}{\pi \sqrt{2} j_0(kr)} = \frac{1}{\pi \sqrt{2}} \frac{\sin (kr)}{r}$$

$$\langle k | k' \rangle = \frac{k}{2\pi} \int d^3 \vec{x} |j_0(kr)j_0(k'r)| = \frac{2\pi}{\beta} \int_0^\pi dr [\sin (kr) \sin (k'r)] = \delta(k - k')$$

We need only to consider the spherical $s$-wave, because the 3D harmonic oscillator ground state is an $\ell = m = 0$ state and so has a vanishing inner product with spherical harmonic states that do not have $\ell = m = 0$. Taking inner products of these continuum states with the harmonic oscillator ground state, we have (with $|\vec{k}\rangle = k$ for the plane wave case):

$$\langle 0 | \vec{k} \rangle = \int d^3 \vec{x} \left( \frac{1}{(2\pi)^{3/2}} e^{i\vec{k} \cdot \vec{x}} \left( \frac{2\beta}{\pi} \right)^{3/4} e^{-2\beta \vec{x}^2} \right)$$

$$= \left( \frac{\beta}{2\pi^3} \right)^{3/4} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi \left( r^2 \sin \theta e^{ikr \cos \theta} e^{-r^2} \right)$$

$$= \left( \frac{\beta}{2\pi^3} \right)^{3/4} 2\pi \int_0^\infty dr \left( r^2 e^{-2\beta r^2} \frac{e^{ikr \cos \theta}}{r^2} \right)$$

$$= \left( \frac{\beta}{2\pi^3} \right)^{3/4} \frac{4\pi}{k} \int_0^\infty \left( r \sin (kr) e^{-r^2} \right)$$

$$= \left( \frac{\beta}{2\pi^3} \right)^{3/4} \frac{4\pi}{k} I = \left( \frac{1}{2\pi \beta} \right)^{3/4} e^{-k^2/4\beta}$$

$$\langle 0 | k \rangle = \int d^3 \vec{x} \left( \frac{k}{\pi \sqrt{2}} j_0(kr) \left( \frac{2\beta}{\pi} \right)^{3/4} e^{-\beta r^2} \right)$$

$$= \left( \frac{2\beta}{\pi} \right)^{3/4} \frac{1}{\pi \sqrt{2}} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi \left( r^2 \sin \theta \frac{\sin (kr)}{r} e^{-r^2} \right)$$

$$= \left( \frac{2\beta}{\pi} \right)^{3/4} 2\sqrt{2} \int_0^\infty dr \left( r^2 \sin (kr) e^{-r^2} \right)$$

$$= \left( \frac{2\beta}{\pi} \right)^{3/4} 2\sqrt{2} I = \left( \frac{2}{\pi \beta} \right)^{3/4} \frac{k\sqrt{2\pi}}{2} e^{-k^2/4\beta}$$

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where we have used the following evaluation of the integral:

\[
I = \int_0^\infty dr \left( r^2 \sin (kr) e^{-\beta r^2} \right)
= \left. -\frac{1}{2\beta} \sin (kr) e^{-\beta r^2} \right|_0^\infty + \frac{k}{2\beta} \int_0^\infty dr \left( \cos (kr) e^{-\beta r^2} \right)
= \frac{k}{2\beta} \int_0^\infty dr \left( \cos (kr) e^{-\beta r^2} \right)
= \frac{k}{4\beta} \left( \int_0^\infty dr e^{ikr} e^{-\beta r^2} + \int_{-\infty}^0 dr e^{ikr} e^{-\beta r^2} \right)
= \frac{k}{4\beta} \int_{-\infty}^\infty dr e^{ikr} e^{-\beta r^2} = \frac{k}{4\beta} \int_{-\infty}^\infty dr \left( e^{-\beta(r-ik/2\beta)^2} \right)
= \frac{k^2}{4\beta^3/2} e^{-k^2/4\beta}
\]

Now it remains to find the density of states for \(|\hat{k}\rangle\) and \(|k\rangle\).

For \(|\hat{k}\rangle\), we use \(\rho_f(\hat{k}, E)dEd\hat{k} = d^3\hat{k}\) where \(\hat{k} = \frac{k}{|k|}\) is the direction of the wave vector and \(d\hat{k}\) corresponds to the differential solid angle and \(E = \hbar^2 k^2/2m\) to get:

\[
\rho_f(\hat{k}, E) \frac{k^2 dkd\hat{k}}{dEd\hat{k}} = \frac{k^2 dkd\hat{k}}{k^2 dkd/m} = \frac{mk}{\hbar^2} = \frac{\sqrt{2m^{3/2}}}{\hbar^3} E^{1/2}
\]

Finally, we plug everything into Fermi’s Golden Rule with

\[
|\Psi_0\rangle = |-\rangle \otimes |0\rangle \quad , \quad |\Psi_{\hat{k}}\rangle = |+\rangle \otimes |\hat{k}\rangle
\]

\(\hat{k}_0 = k_0 \hat{k}\) , \(E_0 = \frac{\hbar^2 \omega^2}{2m} = \frac{3}{2} \hbar \omega\)

to get the transition rate:

\[
w(0 \to k_0) = \frac{2\pi}{\hbar} |\langle \Psi_{k_0} | W | \Psi_0 \rangle|^2 \rho_f(E_0) = \frac{2\pi}{\hbar} (\hbar \Omega)^2 |\langle 0 | k_0 \rangle|^2 \rho_f(E_0)
= 2\pi \hbar \Omega^2 \left( \frac{2}{\pi \beta} \right)^{3/2} e^{-k_0^2/2\beta} \frac{\sqrt{m}}{\hbar \sqrt{2}} E_0^{-1/2}
= 2\pi \hbar \Omega^2 \left( \frac{4\hbar}{m \pi \omega} \right)^{3/2} \frac{3m \omega \pi}{2\hbar} e^{-3 \sqrt{m}/2h \sqrt{2}} \left( \frac{3}{2} \hbar \omega \right)^{-1/2}
= \frac{8 \sqrt{3} \Omega^2}{\omega}
\]

Thus, we get the same result whether we use transitions to plane waves or transitions to spherical waves (as expected).
(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).

First consider the evolution of a general gaussian in free space and in a harmonic oscillator system. In free space, a gaussian wave packet simply spreads out, dissipating with time. In the harmonic oscillator potential, a gaussian obeys a periodic evolution (think squeezed states). The frequency of transitions between the positive spin (free potential) and negative spin (harmonic oscillator potential) states are determined by the value of $\Omega$.

In the $\Omega \gg \omega$ limit, there is a rapid transition between the positive and negative spin states. Consequently, the position space wavefunction part of the initial state $|\Psi_0\rangle = |-\rangle \otimes |0\rangle$ remains essentially unchanged for a while, since the spreading effect of being in the positive spin free potential occurs at a rate much slower than the rate at which $W$ flips the spin back from positive to negative. Of course after a long time, the initial state will dissipate, which is the unavoidable effect of coupling to the free potential continuum.

In the $\Omega \ll \omega$ limit, there is a slow transition between the positive and negative states, so the rate at which the gaussian wavepacket spreads out is much higher than the rate at which the spin would flip back from positive to negative. When some of the amplitude of the initial state $|\Psi_0\rangle = |-\rangle \otimes |0\rangle$ leaks into the positive spin free potential, it almost completely dissipates since you would expect almost no harmonic oscillator ground state left by the time it flips back to negative spin. Effectively, the decay rate of the initial state is the same as the transition rate $w$ that we solved for in part (a).

(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.

For states $|s\rangle \otimes |\psi\rangle = |s; \psi\rangle$ in the Hilbert space, the potential

$$\Sigma_+ (\vec{x}) = (+; \vec{x}| \hat{V}_2 |+; \vec{x}) = \begin{cases} +\infty & |x| < a \\ 0 & |x| \geq a \end{cases}$$

$$\Sigma_- (\vec{x}) = (-; \vec{x}| \hat{V}_2 |-; \vec{x}) = \begin{cases} 0 & |x| < a \\ +\infty & |x| \geq a \end{cases}$$

(and spin off-diagonal terms of $\hat{V}_2$ being zero) requires that:

$$\psi(\vec{x}) = \langle \vec{x} | \psi \rangle = 0 \text{ in the region } |\vec{x}| \leq a \text{ for states with } s = +$$

$$\psi(\vec{x}) = \langle \vec{x} | \psi \rangle = 0 \text{ in the region } |\vec{x}| \geq a \text{ for states with } s = -$$

Hence, for any two allowed states with different spin, $|+; \psi\rangle$ and $|-; \phi\rangle$ (with $\psi(\vec{x}) = \langle \vec{x} | \psi \rangle$ vanishing for $|\vec{x}| \leq a$ and $\phi(\vec{x}) = \langle \vec{x} | \phi \rangle$ vanishing for $|\vec{x}| \geq a$), we will have

$$\langle \psi | \phi \rangle = \int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0$$

since no overlap is possible. Together with the fact that $\langle s_1 | \sigma_x | s_2 \rangle = 1 - \delta_{s_1,s_2}$, this implies that

$$\langle +; \psi | \hat{W} | +; \phi \rangle = \hbar \Omega \langle + | \sigma_x | + \rangle \int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0$$

$$\langle +; \psi | \hat{W} | -; \phi \rangle = \hbar \Omega \langle + | \sigma_x | - \rangle \int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0$$

$$\langle -; \psi | \hat{W} | +; \phi \rangle = \hbar \Omega \langle - | \sigma_x | + \rangle \int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0$$

$$\langle -; \psi | \hat{W} | -; \phi \rangle = \hbar \Omega \langle - | \sigma_x | - \rangle \int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0$$

for any allowed $\psi(\vec{x})$ and $\phi(\vec{x})$, and so it follows that the transition rate vanishes, since $\hat{W}$ is effectively zero when the system has potential $\hat{V}_2$.

11.5.19 The Driven Harmonic Oscillator

At $t = 0$ a 1-dimensional harmonic oscillator with natural frequency $\omega$ is driven by the perturbation

$$H_1(t) = -Fx e^{-\Omega t}$$

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 $\omega \neq \Omega$.

First-order:

$$\frac{d\langle f |}{dt} = -\frac{i}{\hbar} \int_{t_0}^{t} dt' \langle f | H'(t') | i \rangle e^{i\omega_{f,i}t'} = 0 \quad i = 0, f = 2$$
Second-order:

\[
d_f^{(2)} = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \sum_n \langle f | H'(t') | n \rangle \langle n | H'(t'') | i \rangle e^{i\omega_f t'} e^{i\omega_i t''}
\]

\[
= \sum_n -\frac{F^2}{\hbar^2} \langle f | x | n \rangle \langle n | x | i \rangle \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' e^{i(\omega_f n - \Omega)t'} e^{i(\omega_i - \Omega)t''}
\]

For the harmonic oscillator,

\[
\langle 2 | x | n \rangle = x_0 \langle 2 | (a + a^\dagger) | n \rangle = x_0 (\sqrt{n} \delta_{2,n-1} + \sqrt{n+1} \delta_{2,n+1})
\]

i.e., the only non-zero term is

\[
\langle 2 | x | 1 \rangle \langle 1 | x | 0 \rangle = x_0^2 (1 \delta_{2,0} + \sqrt{2} \delta_{2,2}) (0 \delta_{1,0} + 1 \delta_{1,1}) = \sqrt{2} x_0^2
\]

So,

\[
d_f^{(2)} = -\frac{F^2}{\hbar^2} \frac{\hbar}{2m\omega} \sqrt{2} \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' e^{i(\omega_f n - \Omega)t'} e^{i(\omega_i - \Omega)t''}
\]

Substituting \(\omega_{20} = 2\omega, \omega_{10} = \omega, \omega_{21} = \omega\), we have (choosing \(t_0 = 0\))

\[
d_f^{(2)} = -\frac{F^2}{2m\omega \hbar} \frac{1}{2(\omega - \Omega)^2} \left( e^{2i(\omega - \Omega)t} - e^{i(\omega - \Omega)t} + 1 \right)
\]

Then, squaring, the probability is

\[
P_{(0 \rightarrow 2)} = |d_f|^2 = \frac{F^4}{2m^2\omega^2 \hbar^2(\omega - \Omega)^4} \left( \frac{3}{2} + \frac{1}{2} \cos [2(\omega - \Omega)t] - 2 \cos [(\omega - \Omega)t] \right)
\]

(b) Now begin again and do the simpler case, \(\omega = \Omega\). Again, find the probability that the oscillator will be in the 2\textsuperscript{nd} excited state \(n = 2\) at time \(t > 0\)

Using

\[
d_f^{(2)} = -\frac{F^2}{2m\omega \hbar} \sqrt{2} \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' e^{i(\omega_f n - \Omega)t'} e^{i(\omega_i - \Omega)t''}
\]

we now have the conditions \(\omega_{21} = \Omega, \omega_{10} = \Omega\), so that (for \(t_0 = 0\))

\[
d_f^{(2)} = -\frac{F^2}{2m\omega \hbar} \sqrt{2} \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' = -\frac{F^2}{2m\omega \hbar} \frac{t^2}{2}
\]

Therefore, the probability is

\[
P_{(0 \rightarrow 2)} = \frac{F^4 t^4}{8\hbar^2 m^2 \omega^2}
\]

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(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.

If we expand, the probability is
\[
P_{(0\rightarrow 2)} \approx \frac{F^4}{2m^2\omega^2\hbar^2(\omega - \Omega)^4} \left( \frac{3}{2} + \left( \frac{1}{2} - (\omega - \Omega)^2 + \frac{(\omega - \Omega)^4}{3} \right) - \frac{2}{2} - (\omega - \Omega)^2 + \frac{(\omega - \Omega)^4}{12} \right)\]
\[
= \frac{F^4 t^4}{8\hbar^2 m^2\omega^2}
\]
which is identical to the result obtained in part (b).

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 \( \alpha = m\omega/\hbar, \omega = \sqrt{k/m} \) and \( m \) is the mass of the electron. Also assume that the mass of the electron in the quantum well is the same as the free electron mass (not always true in solids).

Clearly, we have a harmonic oscillator with Hamiltonian
\[
H = \frac{p^2}{2m} + \frac{1}{2} kx^2
\]

As we know the ground state wave function is \( \psi_0(x) = N_0 e^{-\alpha x^2/2} \) and the corresponding eigenvalue is \( E_0 = \hbar \omega/2 \) where \( k = m\omega^2 \).

(b) Let us define the raising and lowering operators \( \hat{a} \) and \( \hat{a}^+ \) as
\[
\hat{a}^+ = \frac{1}{\sqrt{2}} \left( \frac{d}{dy} - y \right), \quad \hat{a} = \frac{1}{\sqrt{2}} \left( \frac{d}{dy} + y \right)
\]
where \( y = \sqrt{m\omega/\hbar}x \). Find the wavefunction which results from operating on \( \psi_0 \) with \( \hat{a}^+ \) (call it \( \psi_1(x) \)). What is the eigenvalue of \( \psi_1 \) in this quantum well? You can just state the eigenvalue based on your knowledge - there is no need to derive it.

The state \( \psi_1(x) = \hat{a}^+ \psi_0(x) \) is the first excited state and its energy eigenvalue is \( E_1 = 3\hbar \omega/2 \).
(c) Write down the Fermi’s Golden Rule expression for the rate of a transition
(induced by an oscillating perturbation from electromagnetic radiation)
occurring between the lowest energy eigenstate and the first excited state.
State the assumptions that go into the derivation of the expression.

This is a harmonic perturbation, which is derived in the text. We have
(eq 11.103)
\[ \Gamma_{0 \rightarrow 1} = \frac{2\pi}{\hbar} \frac{|\langle 1 | \hat{V} | 0 \rangle|^2}{4} \]
See reasoning in Chapter 11.

(d) Given that \( k = 3.0 \text{ kg/s}^2 \), what photon wavelength is required to excite
the electron from state \( \psi_0 \) to state \( \psi_1 \)? 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.

We have
\[ \lambda = \frac{c}{\nu} = \frac{2\pi c}{\omega} = \frac{2\pi c\sqrt{me}}{\sqrt{k}} \]

(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.

\[ \langle 0 | x | 1 \rangle = x_0 \langle 0 | (a + a^+) | 1 \rangle = x_0 \]

Thus,
\[ \Gamma_{0 \rightarrow 1} = \frac{2\pi x_0^2}{\hbar} \]

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 \( \alpha \) 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
\[
f(t) = \langle |\Psi(0)\rangle |\Psi(t)\rangle , \quad t \geq 0
\]
Show that \(|f(t)|^2\) is periodic. What is the frequency? How is it related to the
Hamiltonian?

We begin by solving for the eigenstates of the Hamiltonian for \( t \leq 0 \),
\[
H(t \leq 0) = \alpha \begin{pmatrix}
1 & 0 & 1 \\
0 & 2 & 0 \\
1 & 0 & 1
\end{pmatrix}
\]
Clearly, one of the eigenvalues is \( 2\alpha \) with the corresponding eigenstate
\[
\begin{pmatrix}
0 \\
1 \\
0
\end{pmatrix}
\]
Simple algebra on the remaining \( 2 \times 2 \) submatrix gives the other eigenstates as
\[
\frac{1}{\sqrt{2}} \begin{pmatrix}
1 \\
0 \\
1
\end{pmatrix}
\]
with eigenvalue \( 2\alpha \) and
\[
\frac{1}{\sqrt{2}} \begin{pmatrix}
1 \\
0 \\
-1
\end{pmatrix}
\]
with eigenvalue 0 (the ground state). Hence
\[
|\psi(-1)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 \\
0 \\
-1
\end{pmatrix}
\]
and it is a stationary state until time \( t = 0 \). For positive times, we can easily
read off the new energy eigenstates and write
\[
|\psi(t > 0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix}
e^{-i\alpha t} \\
0 \\
e^{-3i\alpha t}
\end{pmatrix}
\]
Then
\[ f(t) = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} e^{-iat} \\ 0 \\ -e^{-3iat} \end{pmatrix} = \frac{1}{2} (e^{-iat} + e^{-3iat}) \]
and therefore
\[ |f(t)|^2 = \frac{1}{2} (1 + \cos(2\alpha t)) \]
which is indeed periodic with the largest Bohr frequency, which is \( 3\alpha - \alpha = 2\alpha \).

11.5.22 The Rabi Formula

Suppose the total Hamiltonian for a spin\(-\frac{1}{2}\) particle is
\[ H = -\gamma [B_0 S_z + b_1 (\cos(\omega t)S_x + \sin(\omega t)S_y)] \]
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
\[ a(0) = 0 \quad b(0) = 1 \]
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.

In the rotating frame
\[ |\psi'(0)\rangle = |\psi(t)\rangle = |-z\rangle \]
and using results from the text (sections on magnetic resonance)
\[ i\hbar \frac{d}{dt} |\psi'(t)\rangle = -\gamma \left( \begin{pmatrix} B_0 + \frac{\omega}{\gamma} S_z + b_1 S_x \end{pmatrix} |\psi'(t)\rangle \right) \]
In matrix representation, we have
\[ \frac{d}{dt} \begin{pmatrix} a \\ b \end{pmatrix} = -i \frac{\Delta}{2} \begin{pmatrix} \Delta & -\gamma b_1 \\ -\gamma b_1 & -\Delta \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \]
and the eigenvalues of the effective Hamiltonian are given by
\[ 0 = \left( -\frac{i\Delta}{2} - \lambda \right) \left( \frac{i\Delta}{2} - \lambda \right) + \frac{1}{4} (\gamma b_1)^2 = \lambda^2 + \frac{1}{4} \Delta^2 + \frac{1}{4} (\gamma b_1)^2 \]
\[ \lambda = \pm \frac{i}{2} \sqrt{\Delta^2 + (\gamma b_1)^2} \]
The corresponding eigenvectors are determined by
\[
\begin{pmatrix}
-i\frac{\Delta}{2} - \lambda & i\frac{\gamma b_1}{2} \\
-i\frac{\Delta}{2} - \lambda & i\frac{\gamma b_1}{2}
\end{pmatrix}
\begin{pmatrix}
a \\
b
\end{pmatrix}
= \begin{pmatrix}
0 \\
0
\end{pmatrix}
\]
or
\[
\begin{pmatrix}
-i\frac{\Delta}{2} - \lambda \\
i\frac{\gamma b_1}{2}
\end{pmatrix}a + i\frac{\gamma b_1}{2}b = 0
\]
or
\[
a = -\frac{\gamma b_1}{i\Delta + 2\lambda}b
\]
Thus, the unnormalized eigenstates and eigenvalues are
\[
|a+\rangle = \begin{pmatrix} i\Delta + i\sqrt{\Delta^2 + (\gamma b_1)^2} \\ -i\gamma b_1 \end{pmatrix} \leftrightarrow +i\frac{\gamma}{2} \sqrt{\Delta^2 + (\gamma b_1)^2}
\]
\[
|a-\rangle = \begin{pmatrix} i\Delta - i\sqrt{\Delta^2 + (\gamma b_1)^2} \\ -i\gamma b_1 \end{pmatrix} \leftrightarrow -i\frac{\gamma}{2} \sqrt{\Delta^2 + (\gamma b_1)^2}
\]
Thus,
\[
\begin{pmatrix}
0 \\
1
\end{pmatrix}
= \frac{1}{2i\sqrt{\Delta^2 + (\gamma b_1)^2}}(|a+\rangle - |a-\rangle)
\]
and so
\[
\begin{pmatrix}
a(t) \\
b(t)
\end{pmatrix}
= \frac{1}{2i\sqrt{\Delta^2 + (\gamma b_1)^2}}(|a+\rangle e^{i\frac{\gamma}{2} \sqrt{\Delta^2 + (\gamma b_1)^2}t} - |a-\rangle e^{-i\frac{\gamma}{2} \sqrt{\Delta^2 + (\gamma b_1)^2}t})
\]
and thus
\[
a(t) = -\frac{i\gamma b_1}{2i\sqrt{\Delta^2 + (\gamma b_1)^2}}(e^{i\frac{\gamma}{2} \sqrt{\Delta^2 + (\gamma b_1)^2}t} - e^{-i\frac{\gamma}{2} \sqrt{\Delta^2 + (\gamma b_1)^2}t})
\]
\[
= -\frac{i\gamma b_1}{2i\sqrt{\Delta^2 + (\gamma b_1)^2}}(2i \sin \left(\frac{\sqrt{\Delta^2 + (\gamma b_1)^2}t}{2}\right))
\]
\[
= -\frac{i\gamma b_1}{\sqrt{\Delta^2 + (\gamma b_1)^2}} \sin \left(\frac{\sqrt{\Delta^2 + (\gamma b_1)^2}t}{2}\right)
\]
and finally,
\[
|a(t)|^2 = \frac{(\gamma b_1)^2}{\Delta^2 + (\gamma b_1)^2} \sin^2 \left(\frac{t}{2} \sqrt{\Delta^2 + (\gamma b_1)^2}\right)
\]

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:

\[
\begin{align*}
|E_0\rangle &= |g\rangle \otimes |0\rangle \\
|E_{1+}\rangle &= \frac{1}{\sqrt{2}} \left( (|g\rangle \otimes |1\rangle) + |e\rangle \otimes |0\rangle \right) \\
|E_{1-}\rangle &= \frac{1}{\sqrt{2}} \left( (|g\rangle \otimes |1\rangle) - |e\rangle \otimes |0\rangle \right) \\
|E_{2+}\rangle &= \frac{1}{\sqrt{2}} \left( (|g\rangle \otimes |2\rangle) + |e\rangle \otimes |1\rangle \right) \\
|E_{2-}\rangle &= \frac{1}{\sqrt{2}} \left( (|g\rangle \otimes |2\rangle) - |e\rangle \otimes |1\rangle \right)
\end{align*}
\]

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

It is immediately clear that \( H_{ac} |E_0\rangle = 0 \), so that it is an eigenstate with eigenvalue zero. Going down the rest of the list

\[
\begin{align*}
H_{ac} |E_{1+}\rangle &= \frac{\hbar \nu}{\sqrt{2}} (|e\rangle \otimes |0\rangle + |g\rangle \otimes |1\rangle) = \hbar \nu |E_{1+}\rangle \rightarrow E_{1+} = \hbar \nu \\
H_{ac} |E_{1-}\rangle &= \frac{\hbar \nu}{\sqrt{2}} (|e\rangle \otimes |0\rangle - |g\rangle \otimes |1\rangle) = -\hbar \nu |E_{1+}\rangle \rightarrow E_{1-} = -\hbar \nu \\
H_{ac} |E_{2+}\rangle &= \frac{\hbar \nu}{\sqrt{2}} (\sqrt{2} |e\rangle \otimes |1\rangle + \sqrt{2} |g\rangle \otimes |2\rangle) = \sqrt{2} \hbar \nu |E_{2+}\rangle \rightarrow E_{2+} = \sqrt{2} \hbar \nu
\end{align*}
\]
\[
H_{ac} |E_{2-}\rangle = \frac{\hbar \nu}{\sqrt{2}} (|e\rangle \otimes |1\rangle - \sqrt{2} |g\rangle \otimes |2\rangle) = -\sqrt{2} \hbar \nu |E_{1+}\rangle \rightarrow E_{2-} = -\sqrt{2} \hbar \nu
\]

By inspection we can write
\[
|\psi(0)\rangle = |g\rangle \otimes (c_0 |0\rangle + c_1 |1\rangle + c_2 |2\rangle) = c_0 |E_0\rangle + \frac{c_1}{\sqrt{2}} (|E_{1+}\rangle + |E_{1-}\rangle) + \frac{c_2}{\sqrt{2}} (|E_{2+}\rangle + |E_{2-}\rangle)
\]

(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 \(\Omega_n\) is the \(n\)-photon Rabi frequency.

We can easily propagate the initial state:
\[
|\psi(t)\rangle = c_0 |E_0\rangle + \frac{c_1}{\sqrt{2}} (e^{-i\nu t} |E_{1+}\rangle + e^{i\nu t} |E_{1-}\rangle) + \frac{c_2}{\sqrt{2}} (e^{-\sqrt{2} i\nu t} |E_{2+}\rangle + e^{\sqrt{2} i\nu t} |E_{2-}\rangle)
\]
and then compute
\[
P_e \otimes I^C |\psi(t)\rangle = \frac{c_1}{2} (e^{-i\nu t} - e^{i\nu t}) |e\rangle \otimes |0\rangle + \frac{c_2}{2} (e^{-\sqrt{2} i\nu t} - e^{\sqrt{2} i\nu t}) |e\rangle \otimes |1\rangle
\]
\[
= -i c_1 \sin (\nu t) |e\rangle \otimes |0\rangle - i c_2 \sin (\sqrt{2} \nu t) |e\rangle \otimes |1\rangle
\]

Using
\[
\langle P_e \rangle = \langle \psi(t) | P_e \otimes I^C | \psi(t) \rangle = (P_e \otimes I^C | \psi(t) \rangle)^* (P_e \otimes I^C | \psi(t) \rangle)
\]
we have
\[
\langle P_e \rangle = |c_1|^2 \sin^2 (\nu t) + |c_2|^2 \sin^2 (\sqrt{2} \nu t)
\]
With \(|c_1|^2 = P(1)\), \(|c_2|^2 = P(2)\) and \(\Omega_n = \nu \sqrt{n}\) we recover the desired expression.
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

\[
\psi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi x}{L} \right)
\]

(a) Find the wavefunctions and energies for the ground state and the first two excited states of the system.

For the single-particle states

\[
E_n = n^2 \frac{\pi^2 \hbar^2}{8ma^2} = \varepsilon n^2
\]

Because this well is not centered on zero, the single-particle eigenstates are given by (choosing \( L = 2a \))

\[
\psi_n(x) = \sqrt{\frac{1}{a}} \sin \left( \frac{n\pi x}{2a} \right) = \langle x | n \rangle
\]

If we write the two-particle states as \( |n_1, n_2\rangle \), the ground-state is \( |1, 1\rangle \) \( (E = 2\varepsilon) \). The first excited states are \( |2, 1\rangle \) \( (E = 5\varepsilon) \) and \( |1, 2\rangle \) \( (E = 5\varepsilon) \). The second excited state is \( |2, 2\rangle \) \( (E = 8\varepsilon) \). The overall wavefunction needs to be symmetric for bosons, which \( |1, 1\rangle \) and \( |2, 2\rangle \) are already. These therefore pair with a symmetric spin wavefunction, which is always possible, whether or not the bosons have spin zero.

For the first excited state, both symmetric and antisymmetric combinations are possible:

\[
\frac{1}{\sqrt{2}} (|2, 1\rangle \pm |1, 2\rangle)
\]
These would need to pair with spin wavefunctions that are symmetric and antisymmetric, respectively. If \( S > 0 \), then both are possible. If \( S = 0 \), then only the symmetric space state is possible.

(b) Suppose that the two bosons interact with each other through the perturbing potential

\[
H'(x_1, x_2) = -L V_0 \delta(x_1 - x_2)
\]

Compute the first-order correction to the ground state energy of the system.

The (normalized) ground-state wavefunction is

\[
\psi(x_1, x_2) = |1, 1\rangle = \frac{1}{a} \sin \left( \frac{\pi x_1}{2a} \right) \sin \left( \frac{\pi x_2}{2a} \right)
\]

According to first-order perturbation theory, the change in the ground-state energy caused by

\[
H'(x_1, x_2) = -2a V_0 \delta(x_1 - x_2)
\]

is

\[
\Delta E = \langle 1, 1 | H'(x_1, x_2) | 1, 1 \rangle = \int \int \psi^*(x_1, x_2) H'(x_1, x_2) \psi(x_1, x_2) dx_1 dx_2
\]

Thus,

\[
\Delta E = -2a V_0 \int \int \psi^*(x_1, x_2) \delta(x_1 - x_2) \psi(x_1, x_2) dx_1 dx_2
\]

\[
= -2a V_0 \int |\psi(x, x)|^2 dx = -2a V_0 \frac{2a}{0} \int \sin^2 \frac{\pi x}{2a} dx = -4V_0 \int \sin^4 \pi y dy
\]

\[
= -4V_0 \int_0^1 \left( \frac{1 - \cos 2\pi y}{2} \right)^2 dy = -4V_0 \frac{3}{8} = \frac{3}{2} V_0
\]

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

\[
u_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n \pi x}{L} \right)
\]

(a) What are the allowed values of the total spin angular momentum quantum number, \( J \)? How many possible values are there for the \( z \)–component of the total angular momentum?
The allowed values of $J$ range between $s_1 + s_2$ and $|s_1 - s_2|$ in integer steps. Since $s_1 = s_2 = 1/2$, the only allowed values are $J = 1$ and $J = 0$. $J = 1$ allows $m = -1, 0, 1$ and $J = 0$ allows $m = 0$ only. Thus, there are only three allowed values of $m$.

(b) If single-particle spin eigenstates are denoted by $|\uparrow\rangle = u$ and $|\downarrow\rangle = d$, construct the two-particle spin states that are either symmetric or antisymmetric. How many states of each type are there?

Symmetric ("triplet") states are

$$u(1)u(2), d(1)d(2) \quad \text{and} \quad \frac{u(1)d(2) + u(2)d(1)}{\sqrt{2}}$$

The antisymmetric ("singlet") state is

$$\frac{u(1)d(2) - u(2)d(1)}{\sqrt{2}}$$

(c) Show that the $j = 1, m = 1$ state must be symmetric. What is the symmetry of the $J = 0$ state?

The $m = 1$ state requires both particles to be spin up. Thus, it must be $J = 1$. We thus need the symmetric state $u(1)u(2)$. The $J = 0$ is antisymmetric.

(d) What is the ground-state energy of the two-particle system, and how does it depend on the overall spin state?

The overall wavefunction of the 2-particle system must be antisymmetric under exchange of spin and space labels (these are fermions). If the wavefunction factorizes into $\psi = u(\text{space}) \times v(\text{spin})$, then the symmetries of $u$ and $v$ must be opposite. Therefore, if $J = 0$ ($v$ is antisymmetric), $u$ must be symmetric, and vice-versa.

A symmetric ground-state is possible:

$$u(1, 2) = u_1(1)u_1(2)$$

but, an antisymmetric space state only allows one particle in the lowest single-particle state allows only one particle in the lowest single-particle state:

$$\frac{u(1)d(2) - u(2)d(1)}{\sqrt{2}}$$

The single-particle energies are

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$
where \( k = \pi / L \) for the \( u_1 \) state and \( k = 2\pi / l \) for the \( u_2 \) state. The symmetric ground-state energy is thus

\[
E_{\text{symm}} = 2 \frac{\hbar^2 (\pi / L)^2}{2m} = \frac{\hbar^2 \pi^2}{mL^2}
\]

whereas the antisymmetric ground state energy is \( 5/2 \) larger, i.e.,

\[
E_{\text{anti}} = \frac{\hbar^2 (\pi / L)^2}{2m} + \frac{\hbar^2 (2\pi / L)^2}{2m} = \left( \frac{1}{2} + 2 \right) \frac{\hbar^2 \pi^2}{mL^2} = \frac{5}{2} E_{\text{symm}}
\]

### 12.9.3 Two spin-1/2 particles

The Hamiltonian for two spin-1/2 particles, one with mass \( m_1 \) and the other with \( m_2 \), is given by

\[
\hat{H} = \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + V_a (r) + \left( \frac{1}{4} - \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2} \right) V_b (r)
\]

where \( |\vec{r}| = |\vec{r}_1 - \vec{r}_2|, |\vec{r}| = r \) and

\[
V_a (r) = \begin{cases} 
0 & \text{for } r < a \\
V_0 & \text{for } r > a 
\end{cases}, \quad V_b (r) = \begin{cases} 
0 & \text{for } r < b \\
V_0 & \text{for } r > b 
\end{cases}
\]

with \( b < a \) and \( V_0 \) very large (assume \( V_0 \) is infinite where appropriate) and positive.

(a) Determine the normalized position-space energy eigenfunction for the ground state. What is the spin state of the ground state? What is the degeneracy?

For a system of 2 spin = 1/2 particles, the eigenstates of \( \vec{S}_1 \cdot \vec{S}_2 \) are the total spin states \( |S, S_z\rangle \) since

\[
\vec{S}_1 \cdot \vec{S}_2 |S, S_z\rangle = \frac{1}{2} \left( \hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2 \right) |S, S_z\rangle = \frac{\hbar^2}{2} \left( S(S + 1) - \frac{3}{2} \right) |S, S_z\rangle
\]

We have allowed total spin values \( S = 0, 1 \) so that

\[
\vec{S}_1 \cdot \vec{S}_2 |1, M\rangle = \frac{\hbar^2}{4} |1, M\rangle, \quad \vec{S}_1 \cdot \vec{S}_2 |0, 0\rangle = -\frac{3\hbar^2}{4} |0, 0\rangle
\]

Since \( [\hat{H}, \vec{S}_1 \cdot \vec{S}_2] = 0 \) we can find simultaneous eigenstates of energy and total spin. This means that for

\[
\hat{H} = \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + V_a (r) + \left( \frac{1}{4} - \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2} \right) V_b (r)
\]

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with

\[ V_a(r) = \begin{cases} 
0 & r < a \\
V_0 & r > a
\end{cases} , \quad V_b(r) = \begin{cases} 
0 & r < b \\
V_0 & r > b
\end{cases} \]

we have

\[
\hat{H} |1, M\rangle = \left( \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + V_a(|r|) + \left( \frac{1}{4} - \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2} \right) V_b(r) \right) |1, M\rangle
\]

\[
\hat{H} |0, 0\rangle = \left( \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + V_a(|r|) + \left( \frac{1}{4} - \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2} \right) V_b(r) \right) |0, 0\rangle
\]

Now we can write

\[
\frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} = \frac{\vec{p}^2}{2M} + \frac{\vec{r}^2}{2M} , \quad \vec{p} = \vec{p}_1 - \vec{p}_2 , \quad \vec{P} = \frac{\vec{p}_1 + \vec{p}_2}{M}
\]

If we choose the CM system, then \( \vec{P} = 0 \) and we have

\[
\hat{H} |1, M\rangle = \left( \frac{\vec{p}^2}{2\mu} + V_a(|r|) \right) |1, M\rangle
\]

\[
\hat{H} |0, 0\rangle = \left( \frac{\vec{p}^2}{2\mu} + V_a(|r|) + V_b(r) \right) |0, 0\rangle
\]

The potentials look like

As \( V_0 \to \infty \), the particles in the spin = 1 states are confined in an infinite potential well of radius \( a \), while the particles in the spin = 0 state are confined in a well of radius \( b \).

Since \( b < a \), the spin = 1 states will have a lower energy \( (1/a^2 < 1/b^2) \) than the spin = 0 state.
To determine the energies, we specify a complete set of 2-particle states in the form \( |E, L, M, S, M_s\rangle \). Then we have

\[
\langle \vec{r}; S = 1, M_s | \hat{H} | E, L, M, S, M_s \rangle = \left[ -\frac{\hbar^2}{2\mu} \left( \frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} \right) + \frac{L(L+1)}{2\mu r^2} R + V_a \right] Y_{LM} = E \rho_{LM} Y_{LM}
\]

The ground state has \( L = 0 \). Now writing \( u = rR \) we have

\[
-\frac{\hbar^2}{2\mu} \frac{d^2 u}{dr^2} + V_a(r) u = Eu \rightarrow \frac{d^2 u}{dr^2} = -\frac{2\mu E}{\hbar^2} u = -k^2 u \quad \text{for} \quad r < a
\]

and \( u = 0 \) for \( r > a \), where the potential barrier is infinite.

Therefore, the ground state wave function for the spin = 1 states is

\[
\langle \vec{r} | E, L = 0, M = 0, S = 1, M_s \rangle = \begin{cases} \frac{1}{\sqrt{\pi}} \sin \frac{n\pi r}{a} Y_{00} |S = 1, M_s\rangle & r < a \\ 0 & r > a \end{cases}
\]

The ground state is 3-fold degenerate.

(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.

The lowest energy spin = 0 state has energy (for \( V_0 \rightarrow \infty \))

\[
E_{n=1} = \frac{\hbar^2 \pi^2}{2\mu b^2}
\]

Since \( b < a \), this is higher than the energy of the spin = 1 states.

The 1\textsuperscript{st} excited states for the spin = 1 states have \( L = 1 \) and therefore

\[
\psi = A j_1(kr)Y_{1M}
\]

for the spatial wave function.

Since \( j_1(ka) = 0 \rightarrow ka = 4.49 \), the lowest energy \( L = 1 \) states (there are 9 such states with \( L = 1, M = 0, \pm 1 \) and \( S = 1, M_s = 0, \pm 1 \) are the first excited states provided that

\[
\frac{\hbar^2(4.49)^2}{2\mu a^2} < \frac{\hbar^2 \pi^2}{2\mu b^2}
\]

or

\[
b < \sqrt{\frac{\pi}{4.49}} a = 0.70a
\]

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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 \( \langle \frac{1}{r} \rangle_{n\ell m} \). We can interpret \( \langle \frac{\lambda}{r} \rangle_{n\ell m} \) as the 1st-order correction due to the perturbation \( \lambda/r \) (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

\[
E(\lambda) = -\frac{m(e^2 - \lambda)^2}{2n^2\hbar^2}
\]

the 1st-order correction is the term linear in \( \lambda \), that is,

\[
E^{(1)} = \frac{me^2\lambda}{n^2\hbar^2} = \langle \frac{\lambda}{r} \rangle_{n\ell m}
\]

Therefore we get

\[
\langle \frac{1}{r} \rangle_{n\ell m} = \frac{me^2}{n^2\hbar^2} = \frac{1}{n^2a_0}
\]

We note (for later use) that

\[
E(\lambda) = E(0) + E^{(1)} + .... = E(\lambda = 0) + \lambda \left( \frac{dE}{d\lambda} \right)_{\lambda=0} + ....
\]

so that one way to extract \( E^{(1)} \) from the exact answer is to calculate

\[
\lambda \left( \frac{dE}{d\lambda} \right)_{\lambda=0}
\]

In order to evaluate \( \langle \frac{1}{r} \rangle \) we consider \( \frac{1}{r} \) as a perturbation for the hydrogenic atom, where we can think of \( \lambda \) as a small constant. The 1st-order shift in the energy is given by

\[
E^{(1)}_n = \langle \frac{\lambda}{r} \rangle_{n\ell m}
\]

which is clearly linear in \( \lambda \). Since the eigenvalues for the Hamiltonian

\[
\hat{H} = \frac{\vec{p}^2}{2\mu} - \frac{Ze^2}{r}
\]

are

\[
E_n = -\frac{\mu Z^2 e^4}{2\hbar^2 n^2}
\]

the eigenvalues of the Hamiltonian

\[
\hat{H} = \frac{\vec{p}^2}{2\mu} - \frac{Ze^2 - \lambda}{r}
\]
are

\[ E_n = -\frac{\mu(Ze^2 - \lambda)^2}{2\hbar^2 n^2} \]

Now, in perturbation theory \( E_n \) is written as a power series in \( \lambda \) so that

\[ E_n^{(1)} = \lambda \left( \frac{dE_n}{d\lambda} \right)_{\lambda=0} \rightarrow E_n^{(1)} = \lambda \frac{Z e^2}{\hbar^2 n^2} \]

However, we also have

\[ E_n^{(1)} = \left\langle \frac{\lambda}{r} \right\rangle_{n\ell m} = \lambda \frac{\mu Z e^2}{\hbar^2 n^2} \rightarrow \left\langle \frac{1}{r} \right\rangle_{n\ell m} = \frac{\mu Z e^2}{\hbar^2 n^2} = \frac{Z}{\alpha_0 n^2} \]

(b) Evaluate, in a manner similar to part (a), \( \left\langle \frac{\hat{p}^2}{2\mu} \right\rangle_{n\ell m} \) by considering the Hamiltonian

\[ \hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{Ze^2}{r} + \lambda \frac{\hat{p}^2}{2\mu} \]

Now we assume the full Hamiltonian is

\[ \hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{Ze^2}{r} + \lambda \frac{\hat{p}^2}{2\mu} = (1 + \lambda) \frac{\hat{p}^2}{2\mu} - \frac{Ze^2}{r} \]

This is the same as a change in the effective mass of the form

\[ \mu \rightarrow \frac{\mu}{1 + \lambda} \]

so that the exact energy eigenvalues become

\[ E_n = -\frac{\mu e^2 Z^2 \alpha^2}{2n^2(1 + \lambda)} \]

and therefore

\[ E_n^{(1)} = \lambda \left( \frac{dE_n}{d\lambda} \right)_{\lambda=0} \rightarrow E_n^{(1)} = \lambda \frac{\mu e^2 Z^2 \alpha^2}{2n^2} = \lambda \left\langle \frac{\hat{p}^2}{2\mu} \right\rangle_{n\ell m} \]

so that

\[ \left\langle \frac{\hat{p}^2}{2\mu} \right\rangle_{n\ell m} = \frac{\mu e^2 Z^2 \alpha^2}{2n^2} \]

(c) Consider now \( \left\langle \frac{\lambda}{r^2} \right\rangle_{n\ell m} \). 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 \( \ell' \) is a function of \( \lambda \). Now go back to the original hydrogen atom solution and show that the dependence of \( E \) on \( \ell'(\lambda) \) is

\[ E(\ell') = -\frac{m e^4}{2\hbar^2 (k + \ell' + 1)^2} = E(\lambda) = E^{(0)} + E^{(1)} + \ldots \]
Then show that
\[
\langle \lambda/r^2 \rangle_{n\ell m} = E^{(1)} \lambda \left( \frac{dE}{d\lambda} \right)_{\lambda=0} = \lambda \left( \frac{dE}{d\ell'} \right)_{\ell'=\ell} \left( \frac{d\ell'}{d\lambda} \right)_{\ell'=\ell}
\]
\[
= \frac{\lambda}{n^3 a_0^2 (\ell + 1/2)}
\]
or
\[
\langle 1/r^2 \rangle_{n\ell m} = \frac{1}{n^3 a_0^2 (\ell + 1/2)}
\]
A perturbation \( \lambda \) modifies the \( 1/r^2 \) term as follows:
\[
\frac{\hbar^2 \ell (\ell + 1)}{2 \mu r^2} + \frac{\lambda}{r^2} = \frac{\hbar^2 \ell' (\ell' + 1)}{2 \mu r^2}
\]
so that
\[
E(\ell') = -\frac{\mu c^2 Z^2 \alpha^2}{2(k + \ell' + 1)^2}
\]
The old quantum number \( n = k + \ell + 1 \).

As above we then have
\[
\langle \lambda/r^2 \rangle_{n\ell m} = E^{(1)} \lambda \left( \frac{dE}{d\lambda} \right)_{\lambda=0} = \lambda \left( \frac{dE}{d\ell'} \right)_{\ell'=\ell} \left( \frac{d\ell'}{d\lambda} \right)_{\ell'=\ell}
\]
Now,
\[
\frac{d}{d\lambda} \left( \frac{\hbar^2 \ell (\ell + 1)}{2 \mu r^2} + \frac{\lambda}{r^2} \right) = \frac{d}{d\lambda} \left( \frac{\hbar^2 \ell (\ell + 1)}{2 \mu r^2} \right)
\]
\[
\frac{1}{r^2} = \frac{\hbar^2 (2\ell'+1)}{2 \mu r^2} \frac{d\ell'}{d\lambda} \bigg|_{\ell' = \ell} = \frac{\mu}{(r+1/2)^2}
\]
Therefore,
\[
\langle 1/r^2 \rangle_{n\ell m} = \frac{\mu c^2 Z^2 \alpha^2}{n^3} \frac{\mu}{(\ell + 1/2)h^2} = \frac{Z^2}{n^3 a_0^2 (\ell + 1/2)}
\]

(d) Finally consider \( \langle \lambda/r^3 \rangle_{n\ell m} \). Since there is no such term in the hydrogen Hamiltonian, we resort to different trick. Consider the radial momentum operator
\[
p_r = -i\hbar \left( \frac{\partial}{\partial r} + \frac{1}{r} \right)
\]
Show that in terms of this operator we may write the radial part of the Hamiltonian
\[
-\frac{\hbar^2}{2m} \left( \frac{1}{r^2} \frac{\partial^2}{\partial r^2} \right)
\]
as
\[
\frac{p_r^2}{2m}
\]
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Now show that
\[ \langle [H, p_r] \rangle = 0 \]
in the energy eigenstates. Using this fact, and by explicitly evaluating the
commutator, show that
\[ \langle 1/r^3 \rangle_{n\ell m} = 0 \]
and hence
\[ \langle 1/r^3 \rangle_{n\ell m} = \frac{Z^3}{n^3a_0^2\ell(\ell + 1)(\ell + 1/2)} \]
Finally,
\[ p_r = -i\hbar \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \]
Therefore,
\[ \frac{p_r^2}{2\mu} f(r) = -\frac{\hbar^2}{2\mu} \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) f(r) = -\frac{\hbar^2}{2\mu} \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \left( \frac{\partial f}{\partial r} + \frac{f}{r} \right) \]
and
\[ \frac{p_r^2}{2\mu} f(r) = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2 f}{\partial r^2} - \frac{f}{r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{1}{r}\frac{f}{r} + \frac{f}{r^2} \right) = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right) f \]
Now, we also have
\[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) f = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial f}{\partial r} \right) = \frac{1}{r^2} \left( 2r \frac{\partial f}{\partial r} + r^2 \frac{\partial^2 f}{\partial r^2} \right) = \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right) f \]
so that
\[ \frac{p_r^2}{2\mu} = -\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \]
Therefore,
\[ \hat{H} = \frac{p_r^2}{2\mu} - \frac{Ze^2}{r} + \frac{\hbar^2\ell(\ell + 1)}{2\mu r^2} \]
Now,
\[ \langle n\ell m | [\hat{H}, \hat{p}_r] | n\ell m \rangle = \langle E_n - E_n \rangle \langle n\ell m | \hat{p}_r | n\ell m \rangle = 0 \]
for all states. But
\[ \langle n\ell m | [\hat{H}, \hat{p}_r] | n\ell m \rangle = \langle n\ell m | \left( \frac{-Ze^2}{r} + \frac{\hbar^2\ell(\ell + 1)}{2\mu r^2} \right) \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) | n\ell m \rangle \]
\[ = \langle n\ell m | \left( \frac{-Ze^2}{r} + \frac{\hbar^2\ell(\ell + 1)}{2\mu r^2} \right) \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) | n\ell m \rangle \]
Therefore,
\[
\left\langle \frac{Ze^2}{r^2} \right\rangle_{n\ell m} = \left\langle \frac{\hbar^2 \ell(\ell + 1)}{\mu r^3} \right\rangle_{n\ell m}
\]
or
\[
\left\langle \frac{1}{r^3} \right\rangle_{n\ell m} = \frac{Z\mu}{\hbar^2 \ell(\ell + 1)} \left\langle \frac{1}{r^2} \right\rangle_{n\ell m} = \frac{Z\mu}{\hbar^2 \ell(\ell + 1)} \frac{Z^2}{n^3 a_0^2(\ell + 1/2)} = \frac{Z^3}{n^3 a_0^2 \ell(\ell + 1)(\ell + 1/2)}
\]

### 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 $^3P_2$. Carbon is $2p^2 \rightarrow S = 0, 1$ and $L = 0, 1, 2$. This give the following table of allowed multiplets:

<table>
<thead>
<tr>
<th>$L$</th>
<th>$S$</th>
<th>$J$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>$^1D_2$</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$^3P_2$</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$^3P_1$</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>$^3P_0$</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>$^1S_2$</td>
</tr>
</tbody>
</table>

Hund’s rule then says that

- **Maximum** $S \rightarrow S = 1 \rightarrow ^3P_2, ^3P_1, ^3P_0$
- **Maximum** $L \rightarrow L = 1 \rightarrow ^3P_2, ^3P_1, ^3P_0$
- **Maximum** $J \rightarrow J = 0 \rightarrow ^3P_0$ (less than half-filled shell)

so that the ground state of carbon is $^3P_0$. Oxygen is $2p^4 \rightarrow S = 0, 1$ and $L = 0, 1, 2$. This give the following table of allowed multiplets (same as for carbon):

<table>
<thead>
<tr>
<th>$L$</th>
<th>$S$</th>
<th>$J$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>$^1D_2$</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$^3P_2$</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$^3P_1$</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>$^3P_0$</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>$^1S_2$</td>
</tr>
</tbody>
</table>
Hund’s rule then says that

\[ \text{Maximum } S \rightarrow S = 1 \rightarrow {}^3P_2, {}^3P_1, {}^3P_0 \]

\[ \text{Maximum } L \rightarrow L = 1 \rightarrow {}^3P_2, {}^3P_1, {}^3P_0 \]

\[ \text{Maximum } J \rightarrow J = 2 \rightarrow {}^3P_2 \text{ (more than half - filled shell)} \]

so that ground state 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?

Following the methods described in Chapter 12 we have for the \( p^3 \) configuration where \( \ell_1 = \ell_2 = \ell_3 = 1 \) and \( s_1 = s_2 = s_3 = 1/2 \) we have the state table:

<table>
<thead>
<tr>
<th>Entry</th>
<th>( m_\ell = -1 )</th>
<th>( m_\ell = 0 )</th>
<th>( m_\ell = +1 )</th>
<th>( M_L )</th>
<th>( M_S )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>↑↓</td>
<td>↑</td>
<td>-2</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>↑↓</td>
<td>↓</td>
<td>-2</td>
<td>-1/2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>↑↓</td>
<td>↑</td>
<td>-1</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>↑↓</td>
<td>↓</td>
<td>-1</td>
<td>-1/2</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>↑</td>
<td>↑↓</td>
<td>-1</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>↓</td>
<td>↑↓</td>
<td>-1</td>
<td>-1/2</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>↑↓</td>
<td>↑</td>
<td>1</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>↑</td>
<td>↑↓</td>
<td>1</td>
<td>-1/2</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>↑</td>
<td>↑</td>
<td>1</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>↓</td>
<td>↑</td>
<td>1</td>
<td>-1/2</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>↑</td>
<td>↑</td>
<td>2</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>↓</td>
<td>↑</td>
<td>2</td>
<td>-1/2</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>↑</td>
<td>↑</td>
<td>0</td>
<td>3/2</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>↓</td>
<td>↓</td>
<td>0</td>
<td>-3/2</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>↑</td>
<td>↑</td>
<td>0</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>↑</td>
<td>↓</td>
<td>0</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>↓</td>
<td>↑</td>
<td>0</td>
<td>1/2</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>↓</td>
<td>↓</td>
<td>0</td>
<td>-1/2</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>↓</td>
<td>↑</td>
<td>0</td>
<td>-1/2</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>↑</td>
<td>↓</td>
<td>0</td>
<td>-1/2</td>
<td></td>
</tr>
</tbody>
</table>

so that we have the \( M_L - M_S \) table:
Largest $L$ and $S$ are $L = 2$ and $S = 1/2$ which says that we have a

$^2D$ term

$J = 5/2, 3/2 \rightarrow 6 + 4 = 10$ levels

Therefore we get the new (remaining states) $M_L - M_S$ table:

<table>
<thead>
<tr>
<th>$M_L/M_S$</th>
<th>3/2</th>
<th>1/2</th>
<th>-1/2</th>
<th>-3/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>3</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>-2</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Next largest $L$ and $S$ are $L = 1$ and $S = 1/2$ which says that we have a

$^2P$ term

$J = 3/2, 1/2 \rightarrow 4 + 2 = 6$ levels

Therefore we get the new (remaining states) $M_L - M_S$ table:

<table>
<thead>
<tr>
<th>$M_L/M_S$</th>
<th>3/2</th>
<th>1/2</th>
<th>-1/2</th>
<th>-3/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>-1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Next largest $L$ and $S$ are $L = 0$ and $S = 3/2$ which says that we have a

$^4S$ term

$J = 3/2 \rightarrow 4$ levels

There are no remaining states and thus we are finished.

We therefore have the allowed multiplets

$^2D_{5/2,3/2}$ , $^2P_{3/2,1/2}$ , $^4S_{3/2}$

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The rule for finding the ground state is

- maximum $S$ or multiplicity
- maximum $L$
- maximum $J$ if $J > 1/2 - \text{full}$
- minimum $J$ if $J < 1/2 - \text{full}$

In this case, the first part of the rule gives the ground state as $^4S_{3/2}$ and we are done since there is only one multiplet satisfying this part of the rule.

(b) Repeat this calculation for $p^4$ and show that we get the same result as for $p^2$

For the $p^4$ configuration we get the state table

<table>
<thead>
<tr>
<th>Entry</th>
<th>$m_\ell = -1$</th>
<th>$m_\ell = 0$</th>
<th>$m_\ell = +1$</th>
<th>$M_L$</th>
<th>$M_S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>↑↓</td>
<td>↑↓</td>
<td>↑↓</td>
<td>-2</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>↑↓</td>
<td>↑↓</td>
<td>↑↓</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>↑↓</td>
<td>↑↓</td>
<td>↑↓</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>↑↓</td>
<td>↓↓</td>
<td>↓↓</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>5</td>
<td>↑↓</td>
<td>↑↓</td>
<td>↑↓</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>↑↓</td>
<td>↑↓</td>
<td>↑↓</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>↑↓</td>
<td>↑↓</td>
<td>↑↓</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>↑</td>
<td>↑</td>
<td>↑</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>9</td>
<td>↑</td>
<td>↑</td>
<td>↑</td>
<td>0</td>
<td>-1</td>
</tr>
<tr>
<td>10</td>
<td>↑</td>
<td>↑</td>
<td>↑</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>↑</td>
<td>↑</td>
<td>↑</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>↑</td>
<td>↑</td>
<td>↑</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>13</td>
<td>↑</td>
<td>↑</td>
<td>↑</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>14</td>
<td>↑</td>
<td>↑</td>
<td>↑</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>15</td>
<td>↑</td>
<td>↑</td>
<td>↑</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

which is the same as the state table for the $p^2$ configuration in Chapter 12. Therefore we get the same $M_L - M_S$ table as for $p^2$

<table>
<thead>
<tr>
<th>$M_L/M_S$</th>
<th>1</th>
<th>0</th>
<th>-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>-1</td>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>-2</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

and we get the allowed multiplets

$^1D_2$, $^3P_{0,1,2}$, $^1S_0$
maximum $S \rightarrow ^3P_{0,1,2}$
maximum $L \rightarrow ^3P_{0,1,2}$
maximum $J$ if $> 1/2$ - full $\rightarrow ^3P_2$

so that the ground state is $^3P_2$

**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 $u$s (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 $3 \times 3$ 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.

Note that there are 6 permutations of the 3 colors among the 3 quarks, if no 2 quarks have the same color. The completely antisymmetric combination of 3 colors is:

$$\frac{1}{\sqrt{6}}(|rgb⟩ - |rbg⟩ + |bgr⟩ - |gbr⟩ - |grb⟩)$$

(b) Now that you know the color wave function of the quarks in the proton, write down the spin wave function. You must construct a total spin state $|1/2, 1/2⟩$ total spin angular momentum state from three spin $-1/2$ states where the two up quarks must be in a symmetric state.

To construct the spin wave function, we first note that the 3 spin $-1/2$ quarks must combine in such a way as to give an overall spin $-1/2$ for the proton. Second, since the space wave function is symmetric and the color wave function is antisymmetric, the spin wave function of the 2 up quarks must be symmetric. Thus, the 2 up quarks are in a spin $-1$ state. To give the spin wave function of the proton, we pick the $z-$axis to be along the spin direction. Then the spin state is:

$$|1/2, 1/2⟩ = \sqrt{2/3} |11; 1/2, -1/2⟩ - \sqrt{1/3} |10; 1/2, 1/2⟩$$

(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.

The magnetic moment of the proton in this model is thus:

$$\mu_p = \frac{2}{3}(2\mu_u - \mu_d) + \frac{1}{3}\mu_d = \frac{4}{3}\mu_u - \frac{2}{3}\mu_d$$

Hence,

$$g_p \frac{e}{2m_p} = \frac{4}{3} \frac{2}{3} \frac{e}{2m_u} - \frac{1}{3} \left( \frac{1}{3} \right) \frac{e}{2m_d}$$
With \( g_p = 5.58, m_p = 938 \text{ MeV} \), and \( m_u = m_d \), we obtain

\[
m_u = \frac{2m_p}{g_p} = 336 \text{ MeV}
\]

(d) Finally, use your results to predict the gyromagnetic moment of the neutron (neutron results follow from proton results by interchanging u and d labels) and compare with observation.

The neutron wave function may be obtained from the proton wave function by interchanging the u and d quark labels. Thus

\[
\mu_n = \frac{2}{3} \left( 2 \mu_d - \mu_u \right) + \frac{1}{3} \mu_u = \frac{4}{3} \mu_d - \frac{2}{3} \mu_u
\]

We predict the gyromagnetic moment of the neutron to be:

\[
\frac{\mu_n}{\mu_p} = \frac{4}{3} \mu_d - \frac{2}{3} \mu_u - \frac{2}{3} \mu_d = \frac{4}{3} \left( -\frac{1}{3} \right) - \frac{2}{3} \left( -\frac{1}{3} \right) = -\frac{2}{3}
\]

that is, we predict (neglecting the mass difference), \( g_n = -3.72 \). This may be compared with the observed value of \(-3.83\).

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

\[
\hat{H} = \frac{\vec{p}^2}{2m} + \frac{1}{2} k \rho^2
\]

(a) Find the energy and orbital angular momentum of the ground state and the first three excited states.

A three-dimensional harmonic oscillator (Chapter 9) has energy levels

\[
E_{n_r, \ell} = \hbar \omega (2n_r + \ell + \frac{3}{2}), \quad \omega = \sqrt{\frac{k}{m}}
\]

with

\[
N = 2n_r + \ell, \quad N, n_r = 0, 1, 2, \ldots
\]

\[
\psi_{n_r, \ell, m}(y, \theta, \phi) = y^\ell e^{-\frac{y^2}{2}} L_{n_r}^{\ell+\frac{1}{2}} (y^2) Y_m(\theta, \phi)
\]

\[
r = \rho y, \rho^2 = \frac{k^2}{\hbar^2}
\]

such that

The degeneracy is given by

\[
\frac{(N + 1)(N + 2)}{2}
\]

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For the ground state, \( N = 0, \ell = 0 \) and the energy is

\[
E_0 = E_{00} = \frac{3}{2} \hbar \omega
\]

This level is non-degenerate \((2\ell + 1 = 1)\). For the 1st excited state, \( N = 1, \ell = 1 \) and the energy is

\[
E_1 = E_{01} = \frac{5}{2} \hbar \omega
\]

This level is 3-fold degenerate \((2\ell + 1 = 3)\).

(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.

For spin = 1/2 particles, two particles will fill up a state. Thus, when completely full, the ground state contain 2 particles and the 1st excited states contain a total of 6 particles.

Therefore, the ground state energy of the 8-particle system is

\[
E_0 = 2 \times \frac{3}{2} \hbar \omega + 6 \times \frac{5}{2} \hbar \omega = 18 \hbar \omega
\]

(c) Assume that these particles have a magnetic moment of magnitude \( \mu \). 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.

The Hamiltonian of the system is

\[
\hat{H} = \sum_{i=1}^{8} \left( \frac{\vec{p}_i^2}{2m} + \frac{1}{2} k r_i^2 \right) - \sum_{i=1}^{8} \mu_i \cdot \vec{B} - \frac{e}{2mc} \sum_{i=1}^{8} \vec{L}_i \cdot \vec{B}
\]

\[
+ \frac{e^2}{2mc^2} \sum_{i=1}^{8} \vec{A}_i \cdot \vec{A}_i + \frac{1}{2mc^2} \sum_{i=1}^{8} \int \frac{V(r_i)}{r_i^2} \vec{L}_i \cdot \vec{S}_i
\]

where

\[
V(r_i) = \frac{1}{2} k r_i^2
\]
\[ \nabla \times \vec{A} = \vec{B} \rightarrow \vec{A} = \frac{1}{2} \vec{B} \times \vec{r} \]

is the vector potential. Since the eight particles occupy 2 shells, all shells are full. This says that

\[ S = 0, \; L = 0, \; J = 0 \text{ (total values)} \]

or that

\[ \sum_{i=1}^{8} \vec{\mu}_i \cdot \vec{B} = 0 = \sum_{i=1}^{8} \vec{L}_i \cdot \vec{B} \]

We also have that

\[ \sum_{i=1}^{8} \frac{1}{r_i^2} \frac{dV(r_i)}{dr_i} \vec{L}_i \cdot \vec{S}_i = 0 \]

as is shown below:

The wave functions of the system are the products of the following functions (excluding radial parts)

\[
Y_{00}(\hat{e}_1)Y_{00}(\hat{e}_2) \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_1 \downarrow\rangle_2 - |\uparrow\rangle_2 \downarrow\rangle_1 \right) \\
Y_{11}(\hat{e}_3)Y_{11}(\hat{e}_2) \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_3 \downarrow\rangle_4 - |\uparrow\rangle_4 \downarrow\rangle_3 \right) \\
Y_{10}(\hat{e}_5)Y_{10}(\hat{e}_4) \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_5 \downarrow\rangle_6 - |\uparrow\rangle_6 \downarrow\rangle_5 \right) \\
Y_{1,1}(\hat{e}_7)Y_{1,-1}(\hat{e}_8) \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_7 \downarrow\rangle_8 - |\uparrow\rangle_8 \downarrow\rangle_7 \right)
\]

where

\[ \hat{e}_i = \frac{\vec{r}_i}{r_i} \]

This implies that all individual \( \ell_z \)-values are paired and each pair has \( S = 0 \) (singlet spin state).

The total space wavefunction is symmetric so that the total spin vector must be antisymmetric.

Since

\[
\sigma_{1z} \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_1 \downarrow\rangle_2 - |\uparrow\rangle_2 \downarrow\rangle_1 \right) = \frac{1}{\sqrt{2}} \left( |\downarrow\rangle_1 \uparrow\rangle_2 - |\downarrow\rangle_2 \uparrow\rangle_1 \right) \\
\sigma_{2z} \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_1 \downarrow\rangle_2 - |\uparrow\rangle_2 \downarrow\rangle_1 \right) = \frac{1}{\sqrt{2}} \left( |\downarrow\rangle_1 \uparrow\rangle_2 - |\downarrow\rangle_2 \uparrow\rangle_1 \right)
\]

and so on ..... 

Then taking the scalar product with

\[ \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_1 \downarrow\rangle_2 - |\uparrow\rangle_2 \downarrow\rangle_1 \right)^\dagger \]

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we get
\[ \langle \sigma_1x \rangle = \langle \sigma_2x \rangle = \langle \sigma_1y \rangle = \langle \sigma_2y \rangle = \langle \sigma_1z \rangle = \langle \sigma_2z \rangle = 0 \]

Therefore,
\[ \langle \sigma_1z L_1z + \sigma_2z L_2z \rangle \rightarrow \langle L_1z \rangle \langle \sigma_1z \rangle + \langle L_2z \rangle \langle \sigma_2z \rangle = 0 \]

and so on... Thus, the indicated term is zero. We then have
\[ \hat{H} = \sum_{i=1}^{8} \left( \frac{p_{1i}^2}{2m} + \frac{1}{2} k r_{1i}^2 \right) + \frac{e^2}{2mc^2} \sum_{i=1}^{8} (\vec{B} \times \vec{r}_{1i})^2 \]

which corresponds to 8 free oscillators + an extra term. The ground state energy is then
\[ E_0 = 18\hbar \omega + \frac{e^2}{8mc^2} \sum_{i=1}^{8} (\vec{B} \times \vec{r}_{1i})^2 = 18\hbar \omega + \frac{e^2 B^2}{8mc^2} \sum_{i=1}^{8} \langle r_{1i}^2 \sin^2 \theta_i \rangle \]

and the magnetization is
\[ -\frac{\partial E_0}{\partial B} = \frac{e^2 B}{4mc^2} \sum_{i=1}^{8} \langle r_{1i}^2 \sin^2 \theta_i \rangle = \chi B \]

\[ \chi = \text{susceptibility (diamagnetic)} \]

**12.9.9 2 interacting particles**

Consider two particles of masses \( m_1 \neq m_2 \) interacting via the Hamiltonian
\[ \hat{H} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2} m_1 \omega^2 x_1^2 + \frac{1}{2} m_2 \omega^2 x_2^2 + \frac{1}{2} K (x_1 - x_2)^2 \]

(a) Find the exact solutions.

We let
\[ R = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \]
\[ r = x_1 - x_2 \]

We then have
\[ \frac{d}{dx_1} = \frac{\partial R}{\partial x_1} \frac{dR}{dr} + \frac{\partial r}{\partial x_1} \frac{dr}{dr} = \frac{m_1}{m_1 + m_2} \frac{dR}{dr} + \frac{d}{dr} \]
\[ \frac{d^2}{dx_1^2} = \left( \frac{m_1}{m_1 + m_2} \right)^2 \frac{d^2 R}{dr^2} - \frac{2m_1}{m_1 + m_2} \frac{d}{dr} \frac{dR}{dr} + \frac{d^2}{dr^2} \]

and similarly,
\[ \frac{d^2}{dx_2^2} = \left( \frac{m_2}{m_1 + m_2} \right)^2 \frac{d^2 R}{dr^2} - \frac{2m_2}{m_1 + m_2} \frac{d}{dr} \frac{dR}{dr} + \frac{d^2}{dr^2} \]
In addition,
\[ x_1^2 = R^2 + \frac{2m_2}{m_1 + m_2} R r + \left( \frac{m_2}{m_1 + m_2} \right)^2 r^2 \]
\[ x_2^2 = R^2 - \frac{2m_1}{m_1 + m_2} R r + \left( \frac{m_1}{m_1 + m_2} \right)^2 r^2 \]

Therefore, the Hamiltonian becomes
\[ H = \left( -\frac{\hbar^2}{2M} \frac{d^2}{dR^2} + \frac{1}{2} M \omega^2 R^2 \right) + \left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{1}{2} \mu \left( 1 + \frac{K}{\mu \omega^2} \right) \omega^2 \right) r^2 \]

where
\[ M = m_1 + m_2 = \text{total mass} \quad \mu = \frac{m_1 m_2}{m_1 + m_2} = \text{reduced mass} \]

We thus have two independent harmonic oscillators and we can write
\[ E_{pq} = (p + 1/2) \hbar \omega + (q + 1/2) \hbar \omega \sqrt{1 + \frac{K}{\mu \omega^2}} \quad p, q = 0, 1, 2, 3, \ldots \]

and
\[ \psi_{pq}(R, r) = \psi_p(R) \psi_q(r) = N_p N_q e^{-\alpha_1^2 R^2 / 2} H_p(\alpha_1 R) e^{-\alpha_2^2 r^2 / 2} H_q(\alpha_2 r) \]

where
\[ N_p = \left( \frac{\alpha_1 \sqrt{2\pi p!}}{\alpha_1 \sqrt{2\pi q!}} \right)^{1/2} \quad \alpha_1 = \left( \frac{M \omega}{\hbar} \right)^{1/2} \]
\[ N_q = \left( \frac{\alpha_2 \sqrt{2\pi q!}}{\alpha_2 \sqrt{2\pi p!}} \right)^{1/2} \quad \alpha_2 = \left( \frac{\mu \omega}{\hbar} \right)^{1/2} \left( 1 + \frac{K}{\mu \omega^2} \right)^{1/4} \]

(b) Sketch the spectrum in weak coupling limit \( K << \mu \omega^2 \) where \( \mu \) is reduced mass.

For \( K << \mu \omega^2 \) we have
\[ \left( 1 + \frac{K}{\mu \omega^2} \right)^{1/4} \approx 1 \]

so that
\[ E_{pq} = (p + q + 1) \hbar \omega = (N + 1) \hbar \omega = E_N \quad N = 0, 1, 2, 3, \ldots \]

The energy level(degeneracy) structure looks like:
If $K < \mu \omega^2$ we have

$$ \left(1 + \frac{K}{\mu \omega^2}\right)^{1/4} \approx 1 + \frac{K}{2 \mu \omega^2} $$

so that energy levels with the same $q$ value will move upwards by

$$(q + 1/2) \hbar \omega \left(\frac{K}{2 \mu \omega^2}\right)$$

as we show schematically below.

```
  _____  _____  _____
 _____  _____  _____
 _____  _____
 _____  _____
 _____  _____
```

Clearly, the degeneracies are broken!

**12.9.10 LS versus JJ coupling**

Consider a multielectron atom whose electron configuration is

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$$

(a) To what element does this configuration belong? Is it the ground state or an excited state? Explain.

We have $Z = 32$ which is Germanium. It is an excited state of Germanium. The ground state is

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$$
(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.

We consider two electrons in a $4p^4d$ configuration. Following Chapter 12, in the LS-Coupling scheme we have:

$$\ell_1 = 1, \ell_2 = 2 \rightarrow L = 1, 2, 3$$
$$s_1 = s_2 = \frac{1}{2} \rightarrow S = 0, 1$$
$$3 \otimes 1 \rightarrow J = 4, 3, 2$$
$$3 \otimes 0 \rightarrow J = 3 \rightarrow 7 \text{ states}$$
$$2 \otimes 1 \rightarrow J = 3, 2, 1 \rightarrow 16 \text{ states}$$
$$2 \otimes 0 \rightarrow J = 2 \rightarrow 5 \text{ states}$$
$$1 \otimes 1 \rightarrow J = 2, 1, 0 \rightarrow 9 \text{ states}$$
$$1 \otimes 0 \rightarrow J = 1 \rightarrow 3 \text{ states}$$

or

$$J = 4 \text{ in 1 level}$$
$$J = 3 \text{ in 3 levels}$$
$$J = 2 \text{ in 4 levels}$$
$$J = 1 \text{ in 3 levels}$$
$$J = 0 \text{ in 1 level}$$

We have 12 total levels. The energy diagram looks like:
(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]

In the \( jj \)-coupling scheme this looks like:

Notice that the final \( J \) values are identical, but their arrangement in energy is very different.

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

\[
H = \frac{p_{1z}^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{p_{2z}^2}{2m} + \frac{1}{2}m\omega^2 x_2^2
\]

(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?

We decompose the Hamiltonian into two parts

\[
\hat{H} = \left( \frac{p_{1z}^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 \right) + \left( \frac{p_{2z}^2}{2m} + \frac{1}{2}m\omega^2 x_2^2 \right) = \hat{H}_1 + \hat{H}_2
\]

where

\[
[\hat{H}_1, \hat{H}_2] = 0
\]

This means that we can the simultaneous eigenvectors of \( \hat{H}_1 \) and \( \hat{H}_2 \) by

\[ |n_1 n_2\rangle |s, m_s\rangle \]

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where
\[ |n_1 n_2\rangle = 2 - \text{particle total spatial state} \]
\[ |s, m_s\rangle = 2 - \text{particle total spin state} \]

and
\[ E = (n_1 + n_2 + 1) \hbar \omega \]

The ground state is
\[ |00\rangle |s = 0, m_s = 0\rangle \]

with energy
\[ E_0 = \hbar \omega \]

The 1st excited state has \( E_1 = 2\hbar \omega \) and is 4-fold degenerate. The state vectors are
\[
\frac{1}{\sqrt{2}} (|10\rangle + |01\rangle) |s = 0, m_s = 0\rangle = \frac{1}{\sqrt{2}} (|10\rangle + |01\rangle) \left( \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right) \\
= (\text{symmetric})(\text{antisymmetric}) = \text{antisymmetric}
\]
\[
\frac{1}{\sqrt{2}} (|10\rangle - |01\rangle) |s = 1, m_s = 1\rangle = \frac{1}{\sqrt{2}} (|10\rangle - |01\rangle) (|\uparrow\uparrow\rangle) \\
= (\text{antisymmetric})(\text{symmetric}) = \text{antisymmetric}
\]
\[
\frac{1}{\sqrt{2}} (|10\rangle - |01\rangle) |s = 1, m_s = 0\rangle = \frac{1}{\sqrt{2}} (|10\rangle - |01\rangle) \left( \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \right) \\
= (\text{antisymmetric})(\text{symmetric}) = \text{antisymmetric}
\]
\[
\frac{1}{\sqrt{2}} (|10\rangle - |01\rangle) |s = 1, m_s = -1\rangle = \frac{1}{\sqrt{2}} (|10\rangle - |01\rangle) (|\downarrow\downarrow\rangle) \\
= (\text{antisymmetric})(\text{symmetric}) = \text{antisymmetric}
\]

(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.

If the 2 particles interact with the potential energy function above, then the energy of the 2 particles will be lowered when the two particles are within a distance \( a \) of each other.

The spatial wave function will have a larger amplitude for particles to
be close together \((x_1 \approx x_2)\) when the spatial wave function is symmetric rather than in the antisymmetric case, which vanishes when \(x_1 \approx x_2\).

Since a symmetric spatial state means we must have an antisymmetric spin state, that is, \(|s = 0, m_s = 0\rangle\), the total spin \(0\) state will have lower energy than the \(|s = 1, m_s = 0, \pm 1\rangle\) states.

This effect is solely due to the Pauli exclusion principle and antisymmetry of the total wavefunction since there is no spin dependent interaction that could lower the energy.

### 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

The unperturbed system can be treated as consisting of 2 separate single-particle systems and the wave functions as a product of the 2 single-particle wave functions.

\[
\psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_1)\psi(\vec{r}_2)
\]

The lowest energy state wave function is thus (particles are not identical)

\[
\psi_0(\vec{r}_1, \vec{r}_2) = \begin{cases} 
\frac{8}{abc} \sin \frac{\pi x_1}{a} \sin \frac{\pi y_1}{b} \sin \frac{\pi z_1}{c} 
\times \sin \frac{\pi x_2}{a} \sin \frac{\pi y_2}{b} \sin \frac{\pi z_2}{c} 
& 0 < x_i < a, 0 < y_i < b, 0 < z_i < c
0
& \text{otherwise}
\end{cases}
\]

corresponding to energy

\[
E_0 = \frac{\hbar^2 \pi^2}{2m} \left( \frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right)
\]

First-order perturbation theory gives an energy correction

\[
\Delta E = \int \psi_0^* (\vec{r}_1, \vec{r}_2) A\delta(\vec{r}_1 - \vec{r}_2) \psi_0 (\vec{r}_1, \vec{r}_2) d^3\vec{r}_1 d^3\vec{r}_2 = A \int |\psi_0 (\vec{r}_1, \vec{r}_1)|^2 d^3\vec{r}_1
\]

\[
= \left( \frac{8}{abc} \right)^2 \int_0^a \int_0^b \int_0^c \sin^4 \frac{\pi x_1}{a} \sin^4 \frac{\pi y_1}{b} \sin^4 \frac{\pi z_1}{c} \, dx_1 \, dy_1 \, dz_1 = \frac{27A}{8abc}
\]

so that (to 1\(^{st}\) order)

\[
E_0 = \frac{\hbar^2 \pi^2}{2m} \left( \frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right) + \frac{27A}{8abc}
\]
(b) identical particles of spin= 0

For a system of identical spin = 0 particles, the total wavefunction must be symmetric under interchange of any pair of particles. Therefore the lowest energy state is

$$\psi_{\text{symmetric}}(\vec{r}_1, \vec{r}_2) = \psi_0(\vec{r}_1, \vec{r}_2) = \psi_{111}(\vec{r}_1)\psi_{111}(\vec{r}_2)$$

where $\psi_{111}(\vec{r}_1)$ is the ground-state (single particle) wave function.

So the calculation is identical to (a) and we have

$$E_{0,\text{symmetric}} = \frac{\hbar^2 \pi^2}{2m} \left( \frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right) + \frac{27A}{8abc}$$

(c) identical particles of spin= 1/2 with spins parallel

For a system of identical spin = 1/2 particles the total wave function must be antisymmetric. Since the spins are parallel (a symmetric spin state) the spatial wave function must be antisymmetric.

Since

$$\frac{1}{a^2} < \frac{1}{b^2} < \frac{1}{c^2}$$

the lowest energy (antisymmetric) state is

$$\psi_{\text{antisymmetric}}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left( \psi_{211}(\vec{r}_1)\psi_{111}(\vec{r}_2) - \psi_{211}(\vec{r}_2)\psi_{111}(\vec{r}_1) \right)$$

where we only need to change index corresponding to the $x$–direction where $|x| < a$ and where $\psi_{211}(\vec{r}_1)$ is the 1st excited-state (single particle) wave function.

Therefore, the unperturbed energy is

$$E_{0,\text{antisymmetric}} = \frac{\hbar^2 \pi^2}{2m} \left( \frac{4}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right)$$

The first-order energy correction is

$$\Delta E = \int \psi_{\text{anti}}^*(\vec{r}_1, \vec{r}_2) A\delta(\vec{r}_1 - \vec{r}_2)\psi_{\text{anti}}(\vec{r}_1, \vec{r}_2) d^3r_1 d^3r_2 = 0$$

since it is the antisymmetric wave function is zero if $\vec{r}_1 = \vec{r}_2$ as required by the delta-function.

Therefore, to 1st order

$$E_{0,\text{antisymmetric}} = \frac{\hbar^2 \pi^2}{2m} \left( \frac{4}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right)$$
12.9.13  2 particles in a square well

Two identical nonrelativistic fermions of mass \( m \), spin \( \frac{1}{2} \) 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.

For the unperturbed potential energy

\[
V(x) = \begin{cases} 
0 & x \in [0, L] \\
\infty & \text{otherwise} 
\end{cases}
\]

the single particle wave functions are

\[
\psi_n(x) = \begin{cases} 
\sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} & x \in [0, L] \\
0 & \text{otherwise} 
\end{cases} \quad n = \text{integer}
\]

The spin vector of a single particle has the form

\[
\begin{pmatrix} a \\ b \end{pmatrix}
\]

Since we do not consider spin-dependent forces, the wave function of the two particles can be written as the product of the spatial part and the spin part.

The spin part \( \chi_{SM} = \chi_S(M) \) is chosen as an eigenstate of \( \vec{S} = \vec{S}_1 + \vec{S}_2 \) and \( S_z = S_{1z} + S_{2z} \), that is,

\[
\vec{S}^2 \chi_{SM} = S(S+1)\hbar^2 \chi_{SM} \quad S_z \chi_{SM} = M\hbar \chi_{SM}
\]

Now,

\( S = 0 \rightarrow \) spin singlet state
\( \rightarrow \) antisymmetric under interchange of particles
\( S = 1 \rightarrow \) spin triplet state
\( \rightarrow \) symmetric under interchange of particles

Symmetrizing and antisymmetrizing the spatial wave functions of the 2-particle system, we have

\[
\psi^S_{nm}(x_1, x_2) = \begin{cases} 
\frac{1}{\sqrt{2}} (\psi_n(x_1)\psi_m(x_2) + \psi_m(x_1)\psi_n(x_2)) & n \neq m \\
\psi_n(x_1)\psi_n(x_2) & n = m 
\end{cases} \quad n = \text{integer}
\]

\[
\psi^A_{nm}(x_1, x_2) = \frac{1}{\sqrt{2}} (\psi_n(x_1)\psi_m(x_2) - \psi_n(x_2)\psi_m(x_1))
\]

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The corresponding energies are

\[ E_{nm} = \frac{\pi^2 \hbar^2}{2mL^2} \left( n^2 + m^2 \right) \quad n, m = 1, 2, 3, \ldots \]

The total wavefunctions, which must be antisymmetric (fermions), are

\[
\psi_{nm}^{A}(x_1, x_2)\chi_{SM}^{S} = \psi_{nm}^{A}(x_1, x_2)\chi_{00}^{S} \\
\psi_{nm}^{S}(x_1, x_2)\chi_{SM}^{A} = \psi_{nm}^{S}(x_1, x_2)\chi_{1M}^{A} \quad M = 0, \pm 1
\]

The three lowest energy states are the following:

1. The ground state has \( n = m = 1 \), which has a symmetric spatial state, and therefore is a spin singlet
   \[ \psi_0 = \psi_{11}^{S}(x_1, x_2)\chi_{00} \rightarrow \text{non-degenerate} \]

2. The first excited state has \( n = 1, m = 2 \) so that
   \[ \psi_1 = \begin{cases} 
   \psi_{12}^{A}(x_1, x_2)\chi_{1M}^{A} & M = 0, \pm 1 \\
   \psi_{12}^{S}(x_1, x_2)\chi_{00}^{S} & n = \text{integer} 
   \end{cases} \]
   which is 4-fold degenerate.

3. The second excited state has \( n = 2, m = 2 \), which has a symmetric spatial state, and therefore is a spin singlet
   \[ \psi_2 = \psi_{22}^{S}(x_1, x_2)\chi_{00} \rightarrow \text{non-degenerate} \]

(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.

Because the perturbation is independent of spin, the calculation of the 1st-order energy correction can be treated as all non-degenerate cases (there are no nonzero off-diagonal matrix elements).

The corrections are

\[
\Delta E_1^A = \int \int dx_1 dx_2 \left| \psi_{12}^{A}(x_1, x_2) \right|^2 V(x_1 - x_2) \\
\Delta E_1^S = \int \int dx_1 dx_2 \left| \psi_{12}^{S}(x_1, x_2) \right|^2 V(x_1 - x_2) \\
\Delta E_2 = \int \int dx_1 dx_2 \left| \psi_{22}^{S}(x_1, x_2) \right|^2 V(x_1 - x_2)
\]

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.

We have the Hamiltonian

\[
\hat{H} = -\frac{\hbar^2}{2M} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + \frac{1}{2} k (x_1^2 + x_2^2) + \frac{1}{2} K (x_1 - x_2)^2
\]

(a) What are the energies of the three lowest states of this system?

We let

\[
\xi = \frac{1}{\sqrt{2}} (x_1 + x_2) \quad \text{and} \quad \eta = \frac{1}{\sqrt{2}} (x_1 - x_2)
\]

and the Hamiltonian becomes

\[
\hat{H} = -\frac{\hbar^2}{2M} \left( \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2} \right) + \frac{1}{2} k \xi^2 + \frac{1}{2} (k + 2K) \eta^2
\]

which corresponds to 2 independent harmonic oscillators with angular frequencies

\[
\omega_1 = \sqrt{\frac{k}{M}} \quad \text{and} \quad \omega_2 = \sqrt{\frac{k + 2K}{M}}
\]

The total energy of the system is

\[
E_{nm} = \left( n + \frac{1}{2} \right) \hbar \omega_1 + \left( m + \frac{1}{2} \right) \hbar \omega_2
\]

and the corresponding eigenfunctions are

\[
|nm\rangle \rightarrow \psi_{nm} = \varphi_n^{(k)}(\xi) \varphi_m^{(k+2K)}(\eta)
\]

where \( n, m = 0, 1, 2, ... \) and \( \varphi_n^{(k)} \) is the \( n^\text{th} \) eigenfunction of a harmonic oscillator with spring constant \( k \).

Thus, the energies of the 3 lowest states of the system are

\[
E_{00} = \frac{1}{2} \hbar (\omega_1 + \omega_2) \quad E_{10} = \frac{1}{2} \hbar (\omega_1 + \omega_2) + \hbar \omega_1 \quad E_{01} = \frac{1}{2} \hbar (\omega_1 + \omega_2) + \hbar \omega_2
\]

(b) If the particles are identical and spinless, which of the states of (a) are allowed?

If the two particles are identical and spinless, the wave function must be symmetric with respect to interchange of the two particles. Thus, the allowed states are

\[
|1\rangle = |00\rangle \quad |2\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle)
\]

which are symmetric.
(c) If the particles are identical and have spin $= 1/2$, which of the states of (a) are allowed?

If the particles are fermions, then the wave functions must be antisymmetric. Thus, the allowed states are

\[ |1\rangle = |00\rangle \text{ spin singlet} \rightarrow \text{non-degenerate} \]
\[ |2\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \text{ spin singlet} \rightarrow \text{non-degenerate} \]
\[ |3\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle) \text{ spin triplet} \rightarrow 3\text{-fold degenerate} \]

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](image)

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.

Given the electron configuration $1s2p$, the total orbital angular momentum is

\[ L = \ell_{1s} + \ell_{2p} = 0 + 1 = 1 \]

so we have a $P$–state. We have the energy level diagram

![Diagram showing energy level splitting](image)

The two-electron state is

\[ |\Psi\rangle = (\text{spatial wave function}) \otimes (\text{spin state}) \]
\[ = \frac{1}{\sqrt{2}} (|\phi_{1s}\rangle |\phi_{2p}\rangle \pm |\phi_{2p}\rangle |\phi_{1s}\rangle) \otimes |\chi_{spin}^T\rangle \]

This is the Fermi symmetry, i.e., symmetric space function with antisymmetric spin state and antisymmetric space function with symmetric spin.
state.

Now we have
\[ |\chi^{-}_{\text{spin}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \] singlet
\[ |\chi^{+}_{\text{spin}}\rangle \begin{cases} |\uparrow\uparrow\rangle \text{ or } \\ |\downarrow\downarrow\rangle \text{ or } \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \end{cases} \] triplet

With a symmetric spatial wave function electrons are (on average) closer together → more repulsion → higher energy. Thus, the singlet is higher energy than the triplet.

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 \( |LM_L M_S \rangle \). What are the good quantum numbers with spin-orbit present?

\( LS \) Coupling: We have \( \hat{H}_{SO} = f(r)\hat{L} \cdot \hat{S} \). The good quantum numbers correspond to the coupled representation of \( \hat{L} \) and \( \hat{S} \), namely,
\[ |JM_J LS \rangle \]

(c) The energy level diagram including spin-orbit corrections is sketched below.

![Figure 12.2: Including Spin-Orbit](image)

Label the states with appropriate quantum numbers. NOTE: Some of the levels are degenerate; the sublevels are not shown.

The possible \( J \) values are \( |L - S| \leq J \leq L + S \). Therefore for the singlet \( S = 0 \), we have \( J = L = 1 \) and for the triplet \( S = 1 \) we have \( J = 2, 1, 0 \). The labelled energy diagram looks like:
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, $\delta_0$, for scattering of low energy particles from the potential

$$ V(r) = \frac{C}{r^4}, \quad C > 0 $$

(a) For low energies, $k \approx 0$, the radial Schrodinger equation for $\ell = 0$ may be approximated by (dropping the energy term):

$$ \left[ -\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{2mC}{\hbar^2 r^4} \right] R^{\ell=0}_{\ell=0}(r) = 0 $$

By making the transformations

$$ R(r) = \frac{1}{\sqrt{r}} \varphi(r), \quad r = \frac{i \sqrt{2mC}}{\hbar} x $$

show that the radial equation may be solved in terms of Bessel functions. Find an approximate solution, taking into account behavior at $r = 0$.

For low energies, $k \approx 0$, the radial Schrodinger equation for $\ell = 0$ may be approximated by dropping the energy term:

$$ \left[ -\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{2mC}{\hbar^2 r^4} \right] R^{\ell=0}_{\ell=0}(r) = 0 $$

By making the transformation

$$ R(r) = \frac{1}{\sqrt{r}} \varphi(r), \quad r = \frac{i \sqrt{2mC}}{\hbar} x $$
we have
\[ \frac{dR}{dr} = \frac{1}{\sqrt{r}} \left( \frac{d\varphi}{dr} - \frac{1}{2r} \varphi \right), \quad \frac{dr}{r} \left( r^2 \frac{dR}{dr} \right) = r^{3/2} \left( \frac{d^2 \varphi}{dr^2} + \frac{1}{r} \frac{d\varphi}{dr} - \frac{1}{4r^2} \varphi \right) \]
so that the radial equation becomes
\[ \frac{d^2 \varphi}{dr^2} + \frac{1}{r} \frac{d\varphi}{dr} - \left( \frac{1}{4r^2} + \frac{2mC}{\hbar^2 r^4} \right) \varphi = 0 \]
and then
\[ \frac{d}{dr} = -\frac{i}{\hbar} \frac{\sqrt{2mC}}{r^2} \frac{d}{dx} = \frac{i\hbar}{\sqrt{2mC}} x^2 \frac{d}{dx} \]
and the radial equation becomes
\[ \left( x^2 \frac{d}{dx} x^2 \frac{d}{dx} - x^3 \frac{d}{dx} + \left( x^4 - \frac{1}{4} x^2 \right) \right) \varphi = 0 \]
or
\[ x^2 \frac{d^2 \varphi}{dx^2} + x \frac{d\varphi}{dx} + \left( x^2 - \frac{1}{4} \right) \varphi = 0 \]
This is Bessel’s equation of half-integer order \( \nu = 1/2 \). Thus, the general solution can be written in terms of spherical Bessel functions
\[ \varphi(x) = AJ_{1/2}(x) + BN_{1/2}(x) = \sqrt{x} (A j_0(x) + B y_0(x)) \]
or spherical Hankel functions
\[ \varphi(x) = \sqrt{x} \left( A h^{(1)}_0(x) + B h^{(2)}_0(x) \right) \]
To understand the behavior of \( \varphi \) as \( r \to \infty \), note that this limit corresponds to \( x \to i\infty \). Since
\[ h^{(1)}_0(x) = -ie^{ix}/x \]
it is converted into a decaying exponential (and hence is safe). \( h^{(2)}_0(x) \), on the other hand, blows up, and should be rejected. So, up to a few constants,
\[ R(r) = \sqrt{x} \varphi(x) = Ax h^{(1)}_0(x) = -iAe^{ix} , \quad x = \frac{i}{\hbar} \sqrt{2mC} r \]
Since the overall normalization is irrelevant, we take simply
\[ R_{\ell=0}^< (r) = e^{-\sqrt{2mC}/hr} \]
So, in the end, this is a very simple result, and no longer even resembles a Bessel function!

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(b) Using the standard procedure of matching this to $R_{\ell=0}^{\text{outside}}(r)$ at $r = a$ (where $a$ is chosen such that $\hbar a \gg \sqrt{2mC}$ and $ka \ll 1$) show that

$$\delta_0 = -k\sqrt{2mC}$$

which is independent of $a$.

We can match at $r = a$ by computing the logarithmic derivative

$$\frac{aR_{\ell=0}'(a)}{R_{\ell=0}(a)} = \beta_0 = \frac{aR_{\ell=0}'(a)}{R_{\ell=0}(a)} = a \frac{d}{dr} \log R_{\ell=0}(r) \bigg|_{r=a} = \frac{\sqrt{2mC}}{\hbar a}$$

Then, as in the text, the phase shift is given by

$$\cot \delta_0 = \frac{ka\eta_0'(ka) - \beta_0\eta_0(ka)}{ka\eta_0'(ka) - \beta_0\eta_0(ka)}$$

Expanding for $ka \ll 1$, we find

$$\cot \delta_0 \approx -\frac{1 + \beta_0}{ka \beta_0} \approx -\frac{1}{ka \beta_0} = -\frac{\hbar}{k\sqrt{2mC}}$$

where we have used the fact that $\hbar a >> \sqrt{2mC}$. Since the expression for $\cot \delta_0$ is very large, this says that

$$\delta_0 \approx -k\sqrt{2mC}$$

We have seen here that, while we had to pick a location $r = a$ to match solutions, in the end the result is independent of $a$, which is physically reasonable.

Of course, if we had a physical barrier at $r = a$ (like a hard sphere or a spherical square well), then the result should depend on $a$. But here $a$ never shows up in the potential $V(r)$, and hence should not show up in the answer!

### 13.3.2 Scattering Slow Particles

Determine the total cross section for the scattering of slow particles ($ka < 1$) by a potential $V(r) = C\delta(r-a)$.

We use the partial wave method. Since $ka << 1$, only $s$-wave scattering is important. We need to find the phase shift $\delta_0$ for $V(r) = C\delta(r-a)$.

We have Region I = $0 \leq r < a$ and Region II = $a < r < \infty$ and $E > 0$. 

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We have for \( u(r) = rR(r) \), the radial equation
\[
\frac{d^2 u(r)}{dr^2} + \frac{2m}{\hbar^2} (E - V(r)) u(r) = 0
\]
In region I the solution is \( u(r) = A \sin kr \), where we have already imposed the boundary condition that \( u(0) = 0 \).

In region II we choose the phase-shifted solution \( u(r) = B \sin (kr + \delta_0) \).

At \( r = a \), we have the boundary conditions
\[
u(r) \text{ is continuous and } \Delta \left( \frac{du}{dr} \right) = \frac{2m}{\hbar^2} Cu(a)
\]
We therefore have
\[
A \sin(ka) = B \sin(ka + \delta_0) \\
ka \cos(ka) = kB \cos(ka + \delta_0) - \frac{2m}{\hbar^2} C \sin(ka)
\]
which gives
\[
k \cot ka + \frac{2m}{\hbar^2} C = k \cot(ka + \delta_0) \\
\delta_0 = \cot^{-1} \left( \cot ka + \frac{2m}{\hbar^2} C \right) - ka
\]
and
\[
\sigma_0 = \frac{4\pi}{k^2} \sin^2 \delta_0
\]

### 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.

The radial wave equation is
\[
\left[ \frac{d^2}{dr^2} + k^2 - U(r) - \frac{\ell(\ell + 1)}{r^2} \right] \chi_{k\ell}(r) = 0
\]
with \( k = \sqrt{2\mu E/\hbar^2} \), \( U(r) = 2\mu g/\hbar^2 r^2 \), and
\[
\psi_{k\ell}(r) Y_{\ell m} = \frac{\chi_{k\ell}(r)}{r} Y_{\ell m}
\]
Substituting the given potential and wavefunction we get
\[
\left[ \frac{d^2}{dr^2} + k^2 - \frac{1}{r^2} \left( \frac{2\mu g}{\hbar^2} + \ell(\ell + 1) \right) \right] \chi_{k1}(r) = 0
\]
For $g = 0$, the solution is given by a free spherical wave

$$
\chi^0_{k_1}(r) = \sqrt{\frac{2k^2r^2}{\pi}} j_k(kr) \rightarrow_{r \to \infty} A \sin(kr - \pi \ell/2)
$$

Therefore, the asymptotic solution for $R_{k_1}(r) = \chi_{k_1}(r)/r$ is

$$
R_{k_1}(r) = A \frac{\sin(kr - \pi \hat{\ell}/2 + \delta_\ell)}{kr} = A \frac{\sin(kr - \pi \tilde{\ell}/2)}{kr}
$$

where $\hat{\ell}$ is given by the relation

$$
\hat{\ell}(\hat{\ell} + 1) = \frac{2\mu g}{\hbar^2} + \ell(\ell + 1)
$$

(b) Prove that the phase shifts are given by

$$
\delta_\ell = \pi \left[ \ell + \frac{1}{2} - \sqrt{\left( \ell + \frac{1}{2} \right)^2 + \frac{2\mu g}{\hbar^2}} \right]
$$

From above we have

$$
\delta_\ell = (\ell - \hat{\ell}) \frac{\pi}{2}
$$

where

$$
\hat{\ell} = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 + 4 \left( \ell(\ell + 1) + \frac{2\mu g}{\hbar^2} \right)} = \frac{1}{2} \pm \sqrt{\frac{1}{4} + \ell(\ell + 1) + \frac{2\mu g}{\hbar^2}}
$$

$$
= \frac{1}{2} + \sqrt{\left( \ell + \frac{1}{2} \right)^2 + \frac{2\mu g}{\hbar^2}}
$$

and we have chosen the $+$ sign so that $\hat{\ell} > 0$. Finally we get

$$
\delta_\ell = \frac{\pi}{2} \left[ \ell + \frac{1}{2} - \sqrt{\left( \ell + \frac{1}{2} \right)^2 + \frac{2\mu g}{\hbar^2}} \right]
$$

(c) Find the energy dependence of the differential cross section for a fixed scattering angle.

The cross section is given by

$$
\frac{d\sigma}{d\Omega} = \frac{1}{k^2} \sum_{\ell=0}^\infty (2\ell + 1)e^{i\delta_\ell} \sin \delta_\ell P_\ell(\cos \theta)
$$

Since the $\delta_\ell$ are not dependent on $k$ (in this particular case), we have

$$
\frac{d\sigma}{d\Omega} \propto \frac{1}{k^2} \propto \frac{1}{E} \Big|_{\theta=\text{constant}}
$$

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(d) Find $\delta_\ell$ for $2\mu g/\hbar^2 \ll 1$ and show that the differential cross section is

$$\frac{d\sigma}{d\theta} = \frac{\pi^3 \, g^2 \mu}{2\hbar^2 \, E} \cot \left( \frac{\theta}{2} \right)$$

where $E$ is the energy of the scattered particle.

For $2\mu g/\hbar^2 \ll 1$ we get

$$\delta_\ell = \frac{\pi}{2} \ell + \frac{1}{2} - \left( \ell + \frac{1}{2} \right) \left[ 1 + \frac{2\mu g}{\hbar^2 \left( \ell + \frac{1}{2} \right)^2} \right]^{1/2}$$

Thus, we have

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2} \left| \sum_{\ell=0}^{\infty} (2\ell + 1) e^{i\delta_\ell} \sin \delta_\ell P_\ell(\cos \theta) \right|^2$$

$$= \frac{1}{k^2} \left| \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{\pi}{2} \frac{\mu g}{\hbar^2 \left( \ell + \frac{1}{2} \right)} P_\ell(\cos \theta) \right|^2$$

$$= \frac{1}{k^2} \left| \sum_{\ell=0}^{\infty} \frac{\pi \mu g}{\hbar^2} P_\ell(\cos \theta) \right|^2 = \frac{\pi^2 \mu^2 g^2}{\hbar^4 k^2} \sum_{\ell=0}^{\infty} P_\ell(\cos \theta)$$

In order to sum the series we use the generating function of $P_\ell(x)$:

$$\sum_{\ell=0}^{\infty} P_\ell(x) y^\ell = \frac{1}{\sqrt{1 - 2x y + y^2}} \Rightarrow \sum_{\ell=0}^{\infty} P_\ell(x) = \frac{1}{\sqrt{2(1-x)}}$$

$$\Rightarrow \sum_{\ell=0}^{\infty} P_\ell(\cos \theta) = \frac{1}{\sqrt{2(1-\cos \theta)}} = \frac{1}{2 \sin(\theta/2)}$$

Therefore,

$$\frac{d\sigma}{d\Omega} = \frac{\pi^2 \mu^2 g^2}{4\hbar^4 k^2} \frac{1}{\sin^2(\theta/2)} = \frac{\pi^2 \mu^2 g^2}{8\hbar^2 E} \frac{1}{\sin^2(\theta/2)}$$

Finally, using $d\Omega = \sin \theta d\theta d\varphi$, we get

$$\frac{d\sigma}{d\theta} = \frac{\pi^3 \mu g^2}{8\hbar^2 E} \sin \theta \frac{\sin \theta}{\sin^2(\theta/2)} \int_0^{2\pi} d\varphi = \frac{\pi^3 \mu g^2}{4\hbar^2 E} \frac{\sin \theta}{\sin^2(\theta/2)}$$

$$= \frac{\pi^3 \mu g^2}{4\hbar^2 E} \frac{2 \sin(\theta/2) \cos(\theta/2) \sin^2(\theta/2)}{\sin^4(\theta/2)} = \frac{\pi^3 \mu g^2}{2\hbar^2 E} \cot(\theta/2)$$

(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?

In the Born approximation, the scattering amplitude is
\[ f_k(\theta, \varphi) = -\frac{1}{4\pi} \int e^{-i\vec{q}\cdot\vec{r}'} U(\vec{r}') d^3r' = -\frac{2\mu g}{\pi \hbar^2} \int \frac{1}{r^2} e^{-i\vec{q}\cdot\vec{r}} d^3r' \]
\[ = -\frac{2\mu g}{\hbar^2} \int_0^\infty \frac{\sin(qr)}{qr} dr = -\frac{\pi \mu g}{\hbar^2 q^2} \]

where \( q = 2k \sin(\theta/2) \). Therefore,
\[ \frac{d\sigma}{d\Omega} = |f_k(\theta, \varphi)|^2 = \frac{\pi^2 \mu^2 g^2}{4\hbar^4 k^2} \frac{1}{\sin^2(\theta/2)} \]

which agrees with our earlier result. This result is expected since all the phase shifts are small.

### 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)?

Note, as \( E \to 0, \ k \to 0, \ ka \to 0 \). If \( ka \ll 1 \), then the scattering is dominated by \( s \)-wave scattering. Then
\[ \sigma_k(\theta) = \frac{1}{k^2} \sin^2 \delta_0, \ \ \sigma_k = \frac{4\pi}{k^2} \sin^2 \delta_0 \]

However, when \( \delta_0 = \pi \), \( \sigma_k(\theta) \) and \( \sigma_k \) are \( \approx 0 \). This is the Ramsauer-Townsend effect. In this case, the \( \ell = 1 \) partial wave contribution to the scattering is the dominant contribution and
\[ \sigma_k(\theta) = \frac{9}{k^2} \sin^2 \delta_1 \cos^2 \theta, \ \ \sigma_k = \frac{12\pi}{k^2} \sin^2 \delta_1 \]

To find the value of \( V_0a^2 \) that gives \( \delta_0 = \pi \), we need to find an expression for \( \delta_0 \) for a 3-dimensional square well potential.

We have
\[ V(r) = \begin{cases} -V_0 & r < a \\ 0 & r > a \end{cases} \]

and
\[ u(r) = \begin{cases} C \sin \sqrt{k^2 + \beta^2} & r < a \\ D \sin (kr + \delta_0) & r > a \end{cases} \]

with
\[ k^2 = \frac{2mE}{\hbar^2}, \ \ \beta^2 = \frac{2mV_0}{\hbar^2} \]
\( u(r) \) and \( du(r)/dr \) are continuous at \( r = a \). This gives
\[
\tan(ka + \delta_0) = \frac{k}{\sqrt{k^2 + \beta^2}} \tan \sqrt{k^2 + \beta^2 a}
\]
We want \( \delta_0 = \pi \). This gives
\[
\tan(ka + \pi) = \tan(ka) = \frac{k}{\sqrt{k^2 + \beta^2}} \tan \sqrt{k^2 + \beta^2 a}
\]
As \( ka \to 0 \), this becomes
\[
ka = \frac{k}{\beta} \tan \beta a \Rightarrow \beta a = n\pi + b
\]
\( n = 0 \), \( b = 0 \) \Rightarrow \( 0 = 0 \)
\( n = 1 \), \( b = 1.352 \) \Rightarrow \( 4.494 \approx 4.497 \)

Thus,
\[
V_0 a^2 = \frac{\hbar^2}{2m} \beta^2 a^2 = \frac{\hbar^2}{2m} (n\pi + b)^2 = \frac{\hbar^2}{2m} (\pi + 1.352)^2 = 10.1 \frac{\hbar^2}{m}
\]

### 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.

The potential created by the dipole is
\[
V(\vec{r}) = -\frac{e^2}{|\vec{r} + \vec{a}|} + \frac{e^2}{|\vec{r} - \vec{a}|}
\]
where we have placed the charge \(-e\) at \(-\vec{a} = -a\hat{x}\) and the charge \(+e\) at \( \vec{a} = a\hat{x}\). The scattering amplitude in Born approximation is
\[
f_{k}(\vec{k}) = -\frac{4\pi^2 m}{\hbar^2} \langle \vec{k} \rangle V(\vec{r}) \langle \vec{k} \rangle = -\frac{4\pi^2 me^2}{\hbar^2} \int \frac{d^3r}{(2\pi)^3} e^{i\vec{r} \cdot \vec{q}} \left( -\frac{1}{|\vec{r} + \vec{a}|} + \frac{1}{|\vec{r} - \vec{a}|} \right)
\]
\[
= -\frac{4\pi^2 me^2}{\hbar^2} \int \frac{d^3r'}{(2\pi)^3} \left( -\frac{e^{i\vec{r}' \cdot \vec{q}} e^{-i\vec{a} \cdot \vec{q}}}{|\vec{r}'|} + \frac{e^{i\vec{r}' \cdot \vec{q}} e^{i\vec{a} \cdot \vec{q}}}{|\vec{r}'|} \right)
\]
\[
= -\frac{4\pi^2 me^2}{\hbar^2} \int \frac{d^3r}{(2\pi)^3} e^{i\vec{r} \cdot \vec{q}} \frac{1}{r} \left( -e^{-i\vec{a} \cdot \vec{q}} + e^{i\vec{a} \cdot \vec{q}} \right)
\]
where \( \vec{q} = \vec{k} - \vec{k}' \), \( q = 2k \sin \frac{\theta}{2} \)

We then have

\[
\int d^3r e^{i\vec{q} \cdot \vec{r}} \frac{1}{r} = 2\pi \int_0^\infty r dr \int_{-1}^1 (d \cos \theta) e^{iqr \cos \theta} = \frac{4\pi}{q^2}
\]

and thus

\[
f_{k}(\vec{k}') = -\frac{4\pi^2 me^2}{\hbar^2} \int \frac{d^3r}{(2\pi)^3} e^{i\vec{q} \cdot \vec{r}} \left( -e^{-i\vec{a} \cdot \vec{q}} + e^{i\vec{a} \cdot \vec{q}} \right)
\]

\[
= -\frac{2me^2}{\hbar^2} \frac{1}{q^2} \left( -e^{-i\vec{a} \cdot \vec{q}} + e^{i\vec{a} \cdot \vec{q}} \right) = -\frac{4ime^2 \sin \vec{a} \cdot \vec{q}}{\hbar^2 q^2}
\]

Letting \( \vec{k} = k \hat{z}, \vec{a} = a \hat{x} \) we have \( \vec{k}' = k \sin \theta \hat{x} + k \cos \theta \hat{z} \), i.e., \( \theta \) is the scattering angle and \( \vec{k}' \) makes an angle \( \theta \) with respect to the \( z \)-direction, we have

\[
q^2 = 2k^2(1 - \cos \theta) \quad , \quad \vec{a} \cdot \vec{q} = -ka \sin \theta
\]

Thus

\[
\sigma_k(\vec{k}') = \left| f_{k}(\vec{k}') \right|^2 = -\frac{4m^2 e^4 \sin^2 (ka \sin \theta)}{(hk)^4 (1 - \cos \theta)^2}
\]

The differential cross-section becomes a maximum when

\[
2a \sin \theta = \frac{\pi}{k} (2n + 1) = \frac{\lambda}{2} (2n + 1)
\]

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 \( V(\vec{r}) = B \delta(\vec{r}) \).

In the Born approximation, we have

\[
\sigma_k(\theta, \varphi) = \frac{m^2}{4\pi^2 \hbar^4} \left| \int d^3r' e^{-i\vec{q} \cdot \vec{r}'} V(\vec{r}') \right|^2
\]

with

\[
\vec{q} = \vec{k} - \vec{k}' \quad , \quad q = 2k \sin \frac{\theta}{2}
\]

Now

\[
\int d^3r' e^{-i\vec{q} \cdot \vec{r}'} V(\vec{r}') = B \int d^3r' e^{-i\vec{q} \cdot \vec{r}'} \delta(\vec{r}) = B
\]

Therefore,

\[
\sigma_k(\theta, \varphi) = \frac{m^2 B^2}{4\pi^2 \hbar^4}
\]

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(b) Comment on the angular and velocity dependence.

Thus, the differential cross-section is independent of scattering angle and the velocity.

(c) Find the total cross section.

The total cross section is then

\[ \sigma_k = \frac{m^2 B^2}{\pi \hbar^4} \]

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.

The translation symmetry of the potential \( V(\vec{r} + \vec{R}) = V(\vec{r}) \), implies

\[ \int e^{-i\vec{q} \cdot \vec{r}} V(\vec{r}) d^3r = \int e^{-i\vec{q} \cdot \vec{r}} V(\vec{r} + \vec{R}) d^3r \]

By changing variables \( \vec{r} \to \vec{r} + \vec{R} \) on the RHS we obtain

\[ \int e^{-i\vec{q} \cdot \vec{r}} V(\vec{r}) d^3r = \int e^{-i\vec{q} \cdot \vec{r}} e^{-i\vec{q} \cdot \vec{R}} V(\vec{r}) d^3r \]

Therefore,

\[ \int e^{-i\vec{q} \cdot \vec{r}} V(\vec{r}) \left[ 1 - e^{-i\vec{q} \cdot \vec{R}} \right] d^3r = \int \left[ 1 - e^{-i\vec{q} \cdot \vec{R}} \right] e^{-i\vec{q} \cdot \vec{r}} V(\vec{r}) d^3r = 0 \]

This holds when either of the following two conditions is satisfied

\[ I \quad \int e^{-i\vec{q} \cdot \vec{r}} V(\vec{r}) d^3r = 0 \quad ( \text{arbitrary } \vec{q}) \]

\[ II \quad e^{-i\vec{q} \cdot \vec{R}} = 1 \to \vec{q} \cdot \vec{R} = 2\pi n \quad (n \text{ is an integer}) \]

Now the Born scattering amplitude is identically zero if I is true. Since this is not the case, we must have condition II satisfied. That completes the proof.

13.3.8 \( \ell = 1 \) hard sphere scattering

Consider the hard sphere potential of the form

\[ V(r) = \begin{cases} 
0 & r > r_0 \\
\infty & r < r_0 
\end{cases} \]
where $kr_0 \ll 1$. Write the radial Schrodinger equation for $\ell = 1$, and show that the solution for the p-wave scattering is of the form

$$\chi_{k1}(r) = rR_{k1}(r) = A \left[ \sin(kr) \frac{kr}{kr} - \cos(kr) + a \left( \cos(kr) \frac{kr}{kr} + \sin(kr) \right) \right]$$

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 $\delta_1(k) \ll \delta_0(k)$.

The radial Schrodinger equation for $r > r_0$ is

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell + 1)}{r^2} \right] \chi_{k\ell}(r) = 0$$

which due to the infinitely repelling potential must be constrained by the condition $\chi_{k\ell}(r_0) = 0$. From my text the general s-wave solution is

$$\chi_{k\ell}(r) = \begin{cases} C_0 \sin k(r - r_0) & r > r_0 \\ 0 & r < r_0 \end{cases}$$

and $\delta_0(k) = -kr_0$ and in the s-wave approximation

$$f_k(\theta) = \frac{1}{r} e^{-ikr_0} \sin(kr_0) \approx r_0 e^{-ikr_0}$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{kr_0^2} \sin^2(kr_0) \approx \frac{r_0^2}{4\pi r_0^2}$$

$$\sigma_{tot} = \frac{4\pi}{k^2} \sin^2(kr_0) \approx 4\pi r_0^2$$

The p-wave radial equation is

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{2}{r^2} \right] \chi_{k1}(r) = 0$$

The general solution is given by

$$\chi_{k1}(r) = c_1 r j_1(kr) + d_1 r n_1(kr)$$

where $j_1(kr)$ and $n_1(kr)$ are spherical Bessel functions

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \quad , \quad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

For $A = c_1/k$, $Aa = -d_1/k$ we obtain

$$\chi_{k1}(r) = A \left[ \sin(kr) \frac{kr}{kr} - \cos(kr) + a \left( \cos(kr) \frac{kr}{kr} + \sin(kr) \right) \right]$$

where $A$ and $a$ are $r$-independent constants.

From the condition $\chi_{k1}(r_0) = 0$, we find

$$a = \frac{\cos(kr_0) - \sin(kr_0)}{\cos(kr_0) + \sin(kr_0)}$$
Furthermore the asymptotic form of $\chi_{k1}(r)$ is

$$
\chi_{k1}(r)_{r \to \infty} = A \left[ - \cos(kr) + a \sin(kr) \right] = C_1 \sin \left( kr - \frac{\pi}{2} + \delta_1 \right)
$$

$$
= C_1 \left[ \sin \left( kr - \frac{\pi}{2} \right) \cos(\delta_1) + \cos \left( kr - \frac{\pi}{2} \right) \sin(\delta_1) \right]
$$

$$
= C_1 \cos(\delta_1) \left[ - \cos (kr) + \sin (kr) \tan(\delta_1) \right]
$$

Identifying $A = C_1 \cos(\delta_1)$ and $a = \tan(\delta_1)$ and using the expression for $a$ above, we get

$$
\tan \delta_1(k) = \frac{\cos(kr_0) - \frac{\sin(kr_0)}{kr_0}}{\cos(kr_0) + \sin(kr_0)}
$$

In the limit $kr_0 << 1$ we have

$$
\sin(kr_0) \approx kr_0 - \frac{(kr_0)^3}{6}, \quad \cos(kr_0) \approx 1 - \frac{(kr_0)^2}{2}
$$

and then

$$
\tan \delta_1(k) \approx 1 - \frac{(kr_0)^2}{2} - 1 + \frac{(kr_0)^2}{6} = -\frac{(kr_0)^3}{2} \Rightarrow \delta_1(k) \approx -\frac{(kr_0)^3}{2}
$$

### 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.

The radial equation describing the motion of the nuclei is

$$
\left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V(r) + \frac{J(J+1)\hbar^2}{2\mu r^2} \right) u_{nJ}(r) = E_{nJ} u_{nJ}(r)
$$

where

$$
V(r) = -2D \left( \frac{a_0}{r} - \frac{a_0^2}{r^2} \right)
$$

The $V(r)$ terms corresponds to vibrational energy and the $J(J+1)$ term corresponds to rotational energy.

To find the extremum for the vibrational energy, we set

$$
\frac{dV(r)}{dr} = 0 \Rightarrow -2D \left( \frac{a_0}{r^2} + \frac{2a_0^2}{r^3} \right) = 0 \Rightarrow r = 2a_0 = r_0
$$
Since, as \( r \to 0 \) \( V(r) \to \infty \) and as \( r \to \infty \) \( V(r) \to 0 \), there is only one extremum and it must be a minimum.

Near \( r_0 \) we can write

\[
V(r) = V(r_0) + \frac{1}{2} \left. \frac{d^2V(r)}{dr^2} \right|_{r_0} (r - r_0)^2
\]

\[
= -2D \left( \frac{a_0}{2a_0} - \frac{a_0^3}{4a_0^3} \right) - \frac{1}{2} 2D \left( \frac{2a_0}{(2a_0)^3} - \frac{6a_0^2}{(2a_0)^4} \right) (r - 2a_0)^2
\]

\[
= -\frac{D}{2} + \frac{D}{8a_0^2} (r - 2a_0)^2 = -V_0 + \frac{1}{2} \mu \omega^2 (r - 2a_0)^2
\]

where

\[
\omega^2 = \frac{D}{4\mu a_0^2}
\]

Therefore, we have a harmonic oscillator with displace origin and frequency \( \omega \).

The vibrational energies are given by

\[
E_n = -V_0 + \hbar \omega (n + 1/2)
\]

The vibrational-rotational energies are given by

\[
E_{nJ} = -V_0 + \hbar \omega (n + 1/2) + \frac{J(J+1)\hbar^2}{8\mu a_0^2}
\]

### 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 \( \text{above} \) and \( \text{below} \) 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 $(|I\rangle, |II\rangle)$

The basis states are

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

To find eigenvalues we solve the characteristic equation

$$\det \left( \begin{pmatrix} E_0 - \lambda & A \\ A & E_0 - \lambda \end{pmatrix} \right) = 0 = (\lambda - (E_0 + A))(\lambda - (E_0 - A))$$

$$\lambda_I = E_0 + A, \quad \lambda_{II} = E_0 - A$$

The corresponding eigenvectors are

$$|I\rangle = \frac{1}{\sqrt{2}} \left( |1\rangle + |2\rangle \right), \quad |II\rangle = \frac{1}{\sqrt{2}} \left( |1\rangle - |2\rangle \right)$$

Thus,

$$|1\rangle = \frac{1}{\sqrt{2}} (|I\rangle + |II\rangle), \quad |2\rangle = \frac{1}{\sqrt{2}} (|I\rangle - |II\rangle)$$

(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?

We have $|\psi(0)\rangle = |I\rangle$. Therefore, since the initial state is an energy eigenvector, we have

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |I\rangle = e^{-i(E_0+A)t/\hbar} |I\rangle = e^{-i(E_0+A)t/\hbar} \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle)$$

and thus

$$P(I) = 1, \quad P(II) = 0, \quad P(1) = P(above) = \frac{1}{2}, \quad P(2) = P(below) = \frac{1}{2}$$

(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?

We have

\(|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|I\rangle + |II\rangle)\)
\(|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |1\rangle = e^{-i(H_0+A)t/\hbar} \frac{1}{\sqrt{2}} (|I\rangle + |II\rangle) = e^{-i(E_0+A)t/\hbar} \frac{1}{\sqrt{2}} |I\rangle + e^{-i(E_0-A)t/\hbar} \frac{1}{\sqrt{2}} |II\rangle\)

Therefore,

\[ P(I) = \frac{1}{2} \quad , \quad P(II) = \frac{1}{2}\]

and

\[ P(1) = P(\text{above}) = \left| e^{-i(E_0+A)t/\hbar} \frac{1}{\sqrt{2}} (1 \langle I | + e^{-i(E_0-A)t/\hbar} \frac{1}{\sqrt{2}} (1 \langle II | \right)^2 \]
\[ = \frac{1}{4} \left| e^{-i(E_0+A)t/\hbar} + e^{-i(E_0-A)t/\hbar} \right|^2 = \cos^2 \left( \frac{At}{\hbar} \right) \]

\[ P(2) = P(\text{below}) = \left| e^{-i(E_0+A)t/\hbar} \frac{1}{\sqrt{2}} (2 \langle I | + e^{-i(E_0-A)t/\hbar} \frac{1}{\sqrt{2}} (2 \langle II | \right)^2 \]
\[ = \frac{1}{4} \left| e^{-i(E_0+A)t/\hbar} - e^{-i(E_0-A)t/\hbar} \right|^2 = \sin^2 \left( \frac{At}{\hbar} \right) \]

13.3.11 Ammonia molecule Redux

Treat the ammonia molecule shown in the figure

![Figure 13.1: Ammonia Molecule](image)

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 \(\hat{L}, I_3\) and \(I_1\).
\[ \hat{H} = \frac{\hat{L}_x^2}{2I_1} + \frac{\hat{L}_y^2}{2I_1} + \frac{\hat{L}_z^2}{2I_3} = \frac{\hat{L}_x^2 - \hat{L}_z^2}{2I_1} + \frac{\hat{L}_z^2}{2I_3} \]

(b) Show that \([\hat{H}, \hat{L}_z] = 0\)

Since \([\hat{L}^2, \hat{L}_z] = 0 = [\hat{L}_z, \hat{L}_z]\), we have \([\hat{H}, \hat{L}_z] = 0\).

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

In addition, we have \([\hat{H}, \hat{L}^2] = 0\) so that the eigenstates of \(\hat{H}\) are the \(|L, M\rangle\) states, that is,

\[ \hat{H} |L, M\rangle = \left( \frac{\hat{L}_x - \hat{L}_y}{2I_1} + \frac{\hat{L}_z}{2I_3} \right) |L, M\rangle = \left( \frac{\hbar^2(L(L+1) - M^2)}{2I_1} + \frac{\hbar^2 M^2}{2I_3} \right) |L, M\rangle \]

\[ \rightarrow E_{L, M} = \frac{\hbar^2(L(L+1) - M^2)}{2I_1} + \frac{\hbar^2 M^2}{2I_3} \]

(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|?

We have

\[ |\psi(0)\rangle = \frac{1}{\sqrt{2}} |0, 0\rangle + \frac{1}{\sqrt{2}} |1, 1\rangle \]

so that

\[ |\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = \frac{1}{\sqrt{2}} e^{-iE_0 t/\hbar} |0, 0\rangle + \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar} |1, 1\rangle = \frac{1}{\sqrt{2}} \left( |0, 0\rangle + e^{-i\hbar \left( \frac{1}{2I_1} + \frac{1}{2I_3} \right) t} |1, 1\rangle \right) \]

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](image)
The eigenstates of the molecule can be written as linear combinations of the atomic states $|\alpha_i\rangle$, $i = 1, 2, 3$, such that

$$
\langle \alpha_i | \hat{H} | \alpha_j \rangle = \begin{cases} 
\varepsilon & \text{if } i = j \\
-\beta & \text{if } i \neq j
\end{cases}
$$

where $\hat{H}$ is the Hamiltonian and $\varepsilon, \beta > 0$. Now define an operator $\hat{R}$ such that

$$
\hat{R} |\alpha_1 \rangle = |\alpha_2 \rangle, \quad \hat{R} |\alpha_2 \rangle = |\alpha_3 \rangle, \quad \hat{R} |\alpha_3 \rangle = |\alpha_1 \rangle
$$

(a) Show that $\hat{R}$ commutes with $\hat{H}$ and find the eigenvalues and eigenvectors of $\hat{R}$.

The three states $|\alpha_i\rangle$ form a complete basis and hence fulfill a completeness relation:

$$
\sum_{j=1}^{3} |\alpha_j \rangle \langle \alpha_j | = \hat{I}
$$

We now have

$$
\langle \alpha_i | (\hat{R} \hat{H} - \hat{H} \hat{R}) | \alpha_k \rangle = \langle \alpha_i | \hat{R} \hat{H} | \alpha_k \rangle - \langle \alpha_i | \hat{H} \hat{R} | \alpha_k \rangle
$$

$$
= \sum_{j=1}^{3} \langle \alpha_i | R | \alpha_j \rangle \langle \alpha_j | H | \alpha_k \rangle - \sum_{j=1}^{3} \langle \alpha_i | H | \alpha_j \rangle \langle \alpha_j | R | \alpha_k \rangle
$$

$$
= \sum_{j=1}^{3} \delta_{i+1,j} \langle \alpha_j | H | \alpha_k \rangle - \sum_{j=1}^{3} \langle \alpha_i | H | \alpha_j \rangle \delta_{j+1,k}
$$

where we use the convenient notation

$$
|\alpha_4 \rangle = |\alpha_1 \rangle, \quad |\alpha_0 \rangle = |\alpha_3 \rangle
$$

Thus,

$$
\langle \alpha_i | (\hat{R} \hat{H} - \hat{H} \hat{R}) | \alpha_k \rangle = \langle \alpha_{i+1} | H | \alpha_k \rangle - \langle \alpha_i | H | \alpha_{k-1} \rangle = \begin{cases} 
\varepsilon - \varepsilon = 0 & \text{if } i + 1 = k \\
(-\varepsilon) - (-\varepsilon) = 0 & \text{if } i + 1 \neq k
\end{cases}
$$

Hence, all matrix elements of the commutator in a complete basis vanish and therefore, $\hat{H}$ and $\hat{R}$ commute.

(b) Find the eigenvalues and eigenvectors of $\hat{H}$.

Since $\hat{H}$ and $\hat{R}$ commute, we can find the eigenvalues and eigenvectors $\hat{R}$ and these will give us the eigenvalues and eigenvectors of $\hat{H}$. For $\hat{R}$, we have the matrix elements

$$
R_{ij} = \begin{cases} 
1 & \text{if } i + 1 = j \\
0 & \text{otherwise}
\end{cases}
$$
We have the characteristic equation

\[ |R - \lambda I| = \begin{vmatrix} -\lambda & 0 & 1 \\ 1 & -\lambda & 0 \\ 0 & 1 & -\lambda \end{vmatrix} = -\lambda^3 + 1 = 0 \]

\[ \Rightarrow \lambda_1 = 1, \; \lambda_2 = e^{i \frac{2\pi}{3}}, \; \lambda_3 = e^{-i \frac{2\pi}{3}} \]

and

\[ \lambda_1 = 1 \Rightarrow \begin{cases} -x_1 + x_3 = 0 \\ x_1 - x_2 = 0 \Rightarrow |X_1| = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \\ x_2 - x_3 = 0 \end{cases} \]

\[ \lambda_2 = e^{i \frac{2\pi}{3}} \Rightarrow \begin{cases} -\lambda_2 x_1 + x_3 = 0 \\ x_1 - \lambda_2 x_2 = 0 \Rightarrow |X_2| = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ \lambda_2^2 \\ \lambda_2 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{i \frac{4\pi}{3}} \\ e^{i \frac{2\pi}{3}} \end{pmatrix} \\ x_2 - \lambda_2 x_3 = 0 \end{cases} \]

\[ \lambda_3 = e^{-i \frac{2\pi}{3}} \Rightarrow \begin{cases} -\lambda_3 x_1 + x_3 = 0 \\ x_1 - \lambda_3 x_2 = 0 \Rightarrow |X_3| = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ \lambda_3^2 \\ \lambda_3 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{-i \frac{4\pi}{3}} \\ e^{-i \frac{2\pi}{3}} \end{pmatrix} \\ x_2 - \lambda_3 x_3 = 0 \end{cases} \]

Since \( H \) and \( R \) commute and \( R \) has a non-degenerate spectrum, they share the set of eigenvectors \( |X_i\rangle \). We then have the \( H \) matrix

\[
H = \begin{pmatrix}
\varepsilon & -t & -t \\
-t & \varepsilon & -t \\
-t & -t & \varepsilon
\end{pmatrix}
\]

and the energy eigenvalues

\[
E_1 = \langle X_1 | H | X_1 \rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}^+ \begin{pmatrix} \varepsilon & -t & -t \\ -t & \varepsilon & -t \\ -t & -t & \varepsilon \end{pmatrix} \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \varepsilon - 2t
\]

\[
E_2 = \langle X_2 | H | X_2 \rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} e^{i \frac{4\pi}{3}} \\ e^{i \frac{2\pi}{3}} \\ 1 \end{pmatrix}^+ \begin{pmatrix} \varepsilon & -t & -t \\ -t & \varepsilon & -t \\ -t & -t & \varepsilon \end{pmatrix} \frac{1}{\sqrt{3}} \begin{pmatrix} e^{i \frac{4\pi}{3}} \\ e^{i \frac{2\pi}{3}} \\ 1 \end{pmatrix} = \varepsilon + t
\]

\[
E_3 = \langle X_3 | H | X_3 \rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} e^{-i \frac{4\pi}{3}} \\ e^{-i \frac{2\pi}{3}} \\ 1 \end{pmatrix}^+ \begin{pmatrix} \varepsilon & -t & -t \\ -t & \varepsilon & -t \\ -t & -t & \varepsilon \end{pmatrix} \frac{1}{\sqrt{3}} \begin{pmatrix} e^{-i \frac{4\pi}{3}} \\ e^{-i \frac{2\pi}{3}} \\ 1 \end{pmatrix} = \varepsilon + t
\]

Thus, \( E_1 = \varepsilon - 2t \) is the ground state, and \( E_2 = E_3 = \varepsilon + t \) is the doubly degenerate excited state.

### 13.3.13 Potential Scattering from a 3D Potential Well

A 3D stepwise constant potential is given by

\[
V(\vec{r}) = \begin{cases}
V_1 & 0 < |\vec{r}| < R_1 \\
V_2 & R_1 < |\vec{r}| < R_2
\end{cases}
\]

and zero outside \( R_2 \).
(1) Calculate the differential cross-section in the Born approximation as a function of the momentum transfer $q$, where $\vec{q} = \vec{k}' - \vec{k}$.

We have

$$f_k(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{-i\vec{q}\cdot\vec{r}} V(\vec{r}) d^3r$$

$$= -\frac{m}{2\pi\hbar^2} \int_0^\infty r^2 V(r) dr 2\pi \int_{-1}^1 d(cos\theta) e^{-iqr\cos\theta}$$

$$= -\frac{m}{\hbar^2} \int_0^\infty r^2 V(r) dr \frac{1}{-iqr} \int_{-iqr}^{iqr} e^x dx$$

$$= -\frac{m}{\hbar^2} \int_0^\infty r^2 V(r) dr \frac{1}{-iqr} (e^{iqr} - e^{-iqr})$$

$$= \frac{2m}{\hbar^2} \int_0^\infty V(r) \sin qr dr$$

$$= \frac{2m}{\hbar^2 q^3} \int_0^\infty V(r) \sin (qr) d(qr)$$

$$= \frac{2m}{\hbar^2 q^3} \left( V_1 \int_0^{qR_1} x \sin x dx + V_2 \int_{qR_1}^{qR_2} x \sin x dx \right)$$

$$= -\frac{2m}{\hbar^2 q^3} (V_1 (F(qR_1) - F(0)) + V_2 (F(qR_2) - F(qR_1)))$$

where

$$F(x) = \sin x - x \cos x$$

Note the limit

$$\lim_{x \to 0} F(x) = \frac{x^3}{3}$$

The differential cross section is

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{4m^2}{\hbar^4 q^6} (V_1 (F(qR_1) - F(0)) + V_2 (F(qR_2) - F(qR_1)))^2$$

(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 $V_1 = V_2 \to V_0$.

The simple square well result, by a similar calculation is

$$\frac{d\sigma}{d\Omega} = \frac{4m^2}{\hbar^4 q^6} (V_0 (F(qR) - F(0)))^2$$

When $V_1 = V_2 = V_0$ and $R_1 = R_2 = R$, our result clearly reduces to that of the simple spherical well.

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(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.

For $y = qR$ we have

$$\frac{d\sigma}{d\Omega} \propto \frac{1}{y^6} (F(y) - F(0))^2 = \frac{1}{y^6} (\sin y - y \cos y)^2$$

A plot looks like

(4) Now plot not simply versus $q$, but versus $\theta$, $0 < \theta < \pi$, 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.

As a function of $\theta$ we have to plot

$$\frac{1}{(2k \sin \frac{\theta}{2} R)^6} \left( \sin (2k \sin \frac{\theta}{2} R) - (2k \sin \frac{\theta}{2} R) \cos (2k \sin \frac{\theta}{2} R) \right)^2$$

where

$$kR = \sqrt{\frac{2mE}{\hbar^2}} \cdot 3a_B = \sqrt{\frac{2\hbar E}{e^2a_0}} \cdot 3a_0 = 3\sqrt{E}$$

with $E$ in Rydbergs. Therefore, we have to plot

$$\frac{1}{(6\sqrt{E} \sin \frac{\theta}{2})^6} \left( \sin \left( 6\sqrt{E} \sin \frac{\theta}{2} \right) - 6\sqrt{E} \sin \frac{\theta}{2} \right) \cos \left( 6\sqrt{E} \sin \frac{\theta}{2} \right)^2$$

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(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.

We set $V_1 = -V_2 = V$ and $R_1 = R$, $R_2 = 2^{1/3} R$. We then have

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{4m^2}{\hbar^2 q^6} V^2 \left( 2F(qR) - F(0) - (F(qR_2) - F(2^{1/3}qR)) \right)^2$$

(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.

Now consider a Gaussian potential

$$V(r) = V_g e^{-r^2/r_0^2}$$

A spherical square well has

$$V(r) = V_{sq} \quad , \quad r < r_0 \quad \text{zero otherwise}$$

The spherical well potential has a volume integral

$$V_{sq} = \frac{4}{3\pi} r_0^3$$

The Gaussian potential has a volume integral

$$4\pi V_g \int_0^\infty e^{-r^2/r_0^2} r^2 dr = V_g \frac{\pi}{3} r_0^3 4\pi$$

If we set the two volume integrals equal, then

$$V_g = \frac{4}{3\sqrt{\pi}} V_{sq}$$

To compare, we look at the ratio

$$\frac{f_{sq}^q}{f_q^q}$$

We have

$$f_{sq}^q = -\frac{2m}{\hbar^2 q^6} (V_{sq}(F(qr_0) - F(0)))$$

For the Gaussian we have

$$f_q^g = -\frac{2m}{\hbar^2} V_g \int_0^\infty r^2 e^{-r^2/r_0^2} \sin qr \frac{qr}{q} dr = -\frac{2m}{\hbar^2} V_g \frac{r_0^2}{q} \frac{1}{4} qr_0 e^{-q^2 r_0^2/4} \sqrt{\pi}$$

$$= -\frac{2m}{\hbar^2} V_g \frac{\sqrt{\pi}}{4} r_0^3 e^{-q^2 r_0^2/4}$$

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Therefore,

\[
\frac{f_{sq}}{f'_{q}} = \frac{-2m}{\hbar^2 q^2} \frac{V_{sq}(F(qr_0) - F(0))}{\frac{2m}{\hbar^2} V_g \frac{\sqrt{\pi}}{4} r_0^3 e^{-q^2 r_0^2/4}} = \frac{3}{(qr_0)^3} (F(qr_0) - F(0)) e^{q^2 r_0^2/4}
\]

Therefore, we have the limit

\[
\lim_{(x=qr_0)\to 0} \frac{f_{sq}}{f'_{q}} = 1
\]

i.e., for low energy the detailed structure does not matter.

### 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.

\[
e = 4\pi \int_0^\infty \rho(r) r^2 dr = 4\pi a \int_0^\infty e^{-br} r^2 dr = \frac{8\pi a}{b^3}
\]

or

\[
1.6 \times 10^{-19} C = 4.8 \times 10^{-10} esu = \frac{8\pi a}{b^3}
\]

which represents one equation for two unknowns. We need to find another equation. Continue to (b) and (c)

(b) Show that the proton mean square radius is given by

\[
\langle r^2 \rangle = \frac{12}{b^2}
\]

Assume that

\[
|\psi(\vec{r})|^2 \propto \rho(r)
\]

Now normalization says that

\[
4\pi \int_0^\infty |\psi(\vec{r})|^2 r^2 dr = 1
\]

Therefore, we have

\[
|\psi(\vec{r})|^2 = \rho(r) \frac{b^3}{8\pi a} = \frac{b^3}{8\pi} e^{-br}
\]
Therefore,

\[
\langle r^2 \rangle = \int r^2 |\psi(\vec{r})|^2 d^3r = 4\pi \int_0^\infty |\psi(\vec{r})|^2 r^4 dr
\]

\[
= \frac{1}{2} b^3 \int_0^\infty r^4 e^{-br} dr = \frac{12}{b^2}
\]

(c) Assuming a reasonable value for \( \langle r^2 \rangle^{1/2} \) calculate \( a \) in esu/cm^2.

Assume that

\[
\sqrt{\langle r^2 \rangle} = 10^{-15} m = 10^{-13} cm
\]

Then we have

\[
b^2 = \frac{12}{\langle r^2 \rangle} = 1.2 \times 10^{27} cm^{-2}
\]

and

\[
a = 4.8 \times 10^{-10} esu \frac{b^3}{8\pi} = 7.9 \times 10^{29} esu - cm^{-3}
\]

### 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

\[
G_E(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} \frac{e^{i\varepsilon k}}{E - \frac{\hbar^2 k^2}{2m} + i\varepsilon}
\]

with \( \varepsilon \) a positive infinitesimal.

To solve the one-dimensional time independent Schrodinger equation

\[
\left( \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + E \right) \psi(x) = V(x)\psi(x)
\]

we define a Green’s function \( G_E(x) \) by

\[
\left( \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + E \right) G_E(x) = \delta(x)
\]

Expressing \( G_E(x) \) and \( \delta(x) \) as Fourier integrals

\[
G_E(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(k) e^{ikx} dk
\]

\[
\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk
\]

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and substituting into the equation for $G_E(x)$ we get
\[
\left( -\frac{\hbar^2 k^2}{2m} + E \right) f(k) = 1 \rightarrow f(k) = \frac{1}{E - \frac{\hbar^2 k^2}{2m}}
\]

As the singularity of $f(k)$ is on the path of integration and the Fourier integral can be understood as an integral in the complex $k$–plane, if we can add $+i\varepsilon$ where $\varepsilon$ is a small positive number, to the denominator of $f(k)$. We then let $\varepsilon \to 0$ after the integration is done.

Consider
\[
G_E(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{E - \frac{\hbar^2 k^2}{2m} + i\varepsilon} e^{ikx} dk
\]

The integral is singular where
\[
E + i\varepsilon - \frac{\hbar^2 k^2}{2m} = 0
\]
that is, at $k = k_1$, where
\[
k_1 = \frac{1}{\hbar} \sqrt{2m(E + i\varepsilon)}
\]

When $x > 0$, the integral becomes a contour integral on the upper half-plane with a singularity at $k = k_1$ with residue
\[
a_1 = -\frac{me^{ik_1z}}{\pi\hbar^2 k_1}
\]
Cauchy’s integral formula then gives
\[
G_E(x) = 2\pi a_1 = -\frac{ime^{ik_1z}}{\hbar^2 k_1}, \quad x > 0
\]
As $\varepsilon \to 0$, $k_1 \to \sqrt{2mE/\hbar}$. This value of $k_1$ can be used in the expression for $G_E(x)$.

Similarly, when $x < 0$, we can carry out the integration along a contour on the lower half-plane and get
\[
G_E(x) = -\frac{ime^{-ik_1z}}{\hbar^2 k_1}, \quad x < 0
\]
Again, we have $k_1 = \sqrt{2mE/\hbar}$.

Thus, the free-particle Green’s function $G_E(x)$ represents an outgoing wave whether $x > 0$ or $x < 0$. 

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(b) Write that the equation for the energy eigenfunction corresponding to an incident wave traveling in the positive $x$-direction. Using this equation find the reflection probability in the first Born approximation for the potential

$$V(x) = \begin{cases} V_0 & |x| < a/2 \\ 0 & |x| > a/2 \end{cases}$$

For what values of $E$ do you expect this to be a good approximation?

The solution of the stationary Schrodinger equation satisfies the integral equation

$$\psi_E(x) = \psi^0(x) + \int_{-\infty}^{\infty} G_E(x - \xi) V(\xi) \psi_E(\xi) d\xi$$

where $\psi^0(x)$ is a solution of the equation

$$\left( \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + E \right) \psi^0(x) = 0$$

In the first-order Born approximation, we replace $\psi^0(x)$ and $\psi_E(x)$ on the RHS of the integral equation by the incident wave function and get

$$\psi_E(x) = e^{ikx} + \int_{-\infty}^{\infty} G_E(x - \xi) V(\xi) e^{ik\xi} d\xi$$

$$= e^{ikx} + \int_{-\infty}^{x} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{ik\xi} d\xi + \int_{x}^{\infty} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{-ik\xi} d\xi + \int_{-\infty}^{x} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{ik\xi} d\xi + \int_{x}^{\infty} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{-ik\xi} d\xi$$

For reflection we require $\psi_E(x)$ for $x \to -\infty$. For $x \to -\infty$

$$\psi_E(x) = e^{ikx} + \int_{-\infty}^{x} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{ik\xi} d\xi$$

$$= e^{ikx} + \int_{-\infty}^{x} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{ik\xi} d\xi + \int_{x}^{\infty} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{-ik\xi} d\xi$$

$$= e^{ikx} + \int_{x}^{\infty} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{-ik(\xi-x)} e^{ik\xi} d\xi = \int_{-\infty}^{a/2} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{-ik(\xi-x)} e^{ik\xi} d\xi$$

$$= \int_{-\infty}^{a/2} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{-ik(\xi-x)} e^{ik\xi} d\xi = \int_{-\infty}^{a/2} (-i) \frac{m}{\hbar^2 k} V(\xi) e^{-ikx} e^{2ik\xi} d\xi$$

Therefore, the reflection probability is

$$R = \frac{|\psi_E(-\infty)|^2}{|\psi_0|^2} = \frac{m^2 V_0^2}{\hbar^4 k^4} \sin^2(ka)$$

When the energy is high,

$$\left| \int_{-\infty}^{\infty} G_E(x - \xi) V(\xi) e^{ik\xi} d\xi \right| << |e^{ikx}| = 1$$
and replacing $\psi(x)$ by $e^{ikx}$ is a good approximation.

13.3.16 Scattering from a Hard Sphere

In this case we have

$$V(x) = \begin{cases} 0 & r > b \\ \infty & r \leq b \end{cases}$$

which is a repulsive potential. Determine the low energy differential and total cross sections. Discuss your results.

In this case we have

$$V(r) = \begin{cases} 0 & r > b \\ \infty & r \leq b \end{cases}$$

This is a repulsive potential. It implies that

$$\psi_0^<(r) = 0 \rightarrow \psi_0^<(b) = \psi_0^>(b) = 0$$

and

$$\alpha_\ell = \infty$$

This gives

$$\cot \delta_\ell = \frac{\eta_\ell(kb)}{j_\ell(kb)}$$

For $\ell = 0$ we have

$$\cot \delta_0 = \frac{\eta_0(kb)}{j_0(kb)} = -\frac{\cos kb}{\sin kb} = -\cot kb$$

or

$$\delta_0 = -kb$$

therefore, for a repulsive potential $\delta_0 < 0$.

What about $\delta_\ell$? Consider low energy or small $k$. We then have for $kb << 1$,

$$\cot \delta_\ell = \frac{\eta_\ell(kb)}{j_\ell(kb)} \approx -\frac{(2\ell-1)!!}{(kb)^{\ell+1}} = -(kb)^{-2\ell-1}(2\ell - 1)!!(2\ell + 1)!!$$

where

$$(2\ell + 1)!! = 1 \cdot 3 \cdot 5 \cdots (2\ell + 1)$$

Therefore, we have

$$\sin \delta_\ell \approx (kb)^{2\ell+1}$$
Thus, we can neglect all terms where $\ell \neq 0$ in the low energy limit and write

$$f(\theta) = \frac{1}{k} P_0(\cos \theta) e^{i \delta_0} \sin \delta_0 = \frac{1}{k} e^{i \delta_0} \sin \delta_0$$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{\sin^2 \delta_0}{k^2} = b^2$$

$$\sigma = 4\pi \frac{\sin^2 \delta_0}{k^2} = 4\pi b^2$$

These results for the hard sphere show that, for low energy, the total cross section is

$$4 \times ( \text{classical scattering cross section})$$

due to quantum interference effects and the scattering is isotropic.

### 13.3.17 Scattering from a Potential Well

In this case

$$V(x) = \begin{cases} 
0 & r > b \\
V_0 & r \leq b 
\end{cases}$$

Determine $\delta_0$, the total cross section and the existence of resonances.

In this case

$$V(r) = \begin{cases} 
0 & r > b \\
-V_0 & r \leq b 
\end{cases}$$

The solution for positive energy inside the well is

$$\psi_\ell^< (r) = j_\ell(qr)$$

where

$$q = \sqrt{\frac{2m}{\hbar^2} (V_0 + E)}$$

Therefore, the boundary conditions at the well edge give

$$\alpha_\ell = \left( \frac{\frac{d}{dr} j_\ell(qr)}{j_\ell(qr)} \right)_{r=b}$$

Now

$$j_0(\rho) = \frac{\sin \rho}{\rho} \quad , \quad j_1(\rho) = \frac{\sin \rho}{\rho^2} - \frac{\cos \rho}{\rho}$$

$$\eta_0(\rho) = -\frac{\cos \rho}{\rho} \quad , \quad \eta_1(\rho) = -\frac{\cos \rho}{\rho^2} - \frac{\sin \rho}{\rho}$$

Therefore,

$$\alpha_0 = q \cot qb - \frac{1}{b}$$

$$\alpha_0 b = qb \cot qb - 1$$
which gives
\[
\cot \delta_0 = \left( \frac{\frac{d\eta_0(kr)}{dr}}{\frac{d\eta_0(kr)}{dr} - \alpha_0 j_0(kr)} \right)_{r=b} = \frac{kb \sin kb + qb \cot qb \cos kb}{kb \cos kb - qb \cot qb \sin kb}
\]
For \( kb < < 1 \) we get
\[
\cot \delta_0 = \frac{qb \cot qb}{kb(1 - qb \cot qb)}
\]
or
\[
\tan \delta_0 = -\frac{kbo_0b}{qb \cot qb} = -\frac{k\alpha_0b^2}{1 + \alpha_0b}
\]
In a similar manner, we can derive
\[
\tan \delta_1 = \frac{(kb)^3}{3} \left( 1 - \frac{\alpha_1 b}{2 + \alpha_1 b} \right)
\]
For low energy \( (k \to 0) \) and a deep well \( (V_0 \text{ large}) \) we get
\[
\sigma = 4\pi b^2 \left( 1 - \frac{\tan qb}{qb} \right)^2
\]
This calculation fails if either
\[
1 + \alpha_0b = 0 \text{ or } 2 + \alpha_1b = 0
\]
which corresponds to the \( \ell = 0 \) or the \( \ell = 1 \) partial wave being in resonance with the potential.

In general, this resonance condition is given by
\[
\ell + 1 + \alpha_\ell b = 0
\]
which implies that
\[
\cot \delta_\ell = 0 \to \tan \delta_\ell = \infty \to \delta_\ell(k) = \left( n + \frac{1}{2} \right) \pi
\]
and thus the partial wave scattering cross section takes on its maximum value, namely,
\[
\sigma_\ell(k) = \frac{4\pi(2\ell + 1)}{k^2}
\]
For other \( k \) values (off-resonance) we have
\[
\delta_\ell \approx (kb)^{2\ell+1}
\]
This says that the resonance is very sharp for large \( \ell \) values.
We can understand this effect better by looking at other features. As we saw, for small $k$, cot $\delta_\ell$ is very large since it is proportional to $k^{-2\ell-1}$. Therefore,

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell + 1)\sin^2 \delta_\ell = \frac{4\pi}{k^2}(2\ell + 1) \frac{1}{1 + \cot^2 \delta_\ell}$$

will be proportional to $k^{4\ell}$. In this case, except for the s-wave ($\ell = 0$), $\sigma_\ell$ will be small.

However, near a resonance energy $E_r$ where

$$\ell + 1 + b\alpha_\ell(E_r) = 0$$

cot $\delta_\ell$ goes to zero and $\sigma_\ell$ will be proportional to $k^{-2}$ and this is quite large (an effect that is called resonance).

Near $E_r$ we can make a Taylor expansion and write

$$\ell + 1 + b\alpha_\ell(E_r) \approx \ell + 1 + b\alpha_\ell(E_r) + (E - E_r)b\left(\frac{\partial \alpha_\ell}{\partial E}\right)_{E=E_r} + ...$$

$$\approx (E - E_r)b\left(\frac{\partial \alpha_\ell}{\partial E}\right)_{E=E_r}$$

and

$$\ell - b\alpha_\ell(E_r) \approx 2\ell + 1$$

After some algebra, these relations imply that

$$\cot \delta_\ell \approx -\frac{2(E - E_r)}{\Gamma_k}$$

where

$$\Gamma_k = -\frac{2k^{2\ell+1}b^{2\ell}}{((2\ell - 1)!!)^2}(\frac{\partial \alpha_\ell}{\partial E})_{E=E_r}$$

Now $\partial \alpha_\ell/\partial E < 0$, which implies that $\Gamma_k > 0$. Therefore, near resonance, the partial wave cross section $\sigma_\ell$ is

$$\sigma_\ell = \frac{4\pi \Gamma_k^2}{4(E - E_r)^2 + \Gamma_k^2}$$

When

$$E - E_r = \pm \frac{\Gamma_k}{2}$$

the partial wave cross section is equal to one-half its maximum value. Therefore, $\Gamma = \Gamma_k(E_r)$ is the width of the resonance at half-maximum.

This functional form is called the *Breit-Wigner* formula for a scattering resonance. The curves are shown in the figure below.

which are standard resonance type curves.

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13.3.18  Scattering from a Yukawa Potential

Use the Born approximation to determine the differential cross section for a Yukawa potential

\[ V(\vec{r}) = a e^{-\mu r} \]

Discuss the limit \( \mu \to 0 \).

In this case

\[ V(r) = a e^{-\mu r} \]

Although this potential is nonzero out to infinity, it is effectively short-range because it falls off exponentially. The effective range is usually given as \( 1/\mu \).

The Fourier transform of this potential is easily calculated to be

\[ \tilde{V}(\vec{k} - \vec{k}') = \frac{4\pi a}{|\vec{k} - \vec{k}'|^2 + \mu^2} \]

where

\[ |\vec{k} - \vec{k}'|^2 = \left(2k \sin \frac{\theta}{2}\right)^2 \]
This gives

\[
\frac{d\sigma}{d\Omega} = \frac{m^2}{(2\pi\hbar^2)^2} \left| \tilde{V}(\vec{k} - \vec{k}') \right|^2 = \frac{m^2}{(2\pi\hbar^2)^2} \left( \frac{4\pi a}{|\vec{k} - \vec{k}'|^2 + \mu^2} \right)^2
\]

\[
= \frac{a^2}{(4E_k \sin^2 \frac{\theta}{2} + \frac{\hbar^2 \mu^2}{2m})^2}
\]

By pure coincidence, if we let \( \mu \to 0 \) so that the Yukawa potential turns into the Coulomb potential we get the result

\[
\frac{d\sigma}{d\Omega} = \frac{a^2}{16E_k^2 \sin^4 \frac{\theta}{2}}
\]

which is the correct Rutherford cross section!

This is an accident and higher order terms will completely change this result. The higher order terms that we have neglected in the Born approximation cannot be ignored for a long-range potential like the Coulomb potential.

Later we will show how to handle Coulomb scattering correctly.

### 13.3.19 Born approximation - Spin-Dependent Potential

Use the Born approximation to determine the differential cross section for the spin-dependent potential

\[
V(\vec{r}) = e^{-\mu r^2} [A + B\vec{\sigma} \cdot \vec{r}]
\]

We now consider the scattering of a particle of mass \( m \) and momentum \( p = \hbar k \) through an angle \( \theta \) by the spin-dependent potential

\[
V(\vec{r}) = e^{-\mu r^2} [A + B\vec{\sigma} \cdot \vec{r}]
\]

where

\[
\vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)
\]

We assume that the initial spin is along the incident direction and we sum over all final spins, which corresponds to measuring only the direction of the scattered particles and not their spins. Note that this potential violates parity.

We use the Born approximation. The Fourier transform of the potential function is given by

\[
\tilde{V}(\vec{q}) = \int d^3\vec{r} V(\vec{r}) e^{-i\vec{q} \cdot \vec{r}}
\]

where

\[
\vec{q} = \vec{k} - \vec{k}'
\]
We get
\[
\tilde{V}(\vec{q}) = \int d^3 r e^{-\mu r^2} [A + B \vec{\sigma} \cdot \vec{r}] e^{-i\vec{q} \cdot \vec{r}}
\]
\[
= \left( \frac{\pi}{\mu} \right)^{3/2} e^{-\frac{\vec{q}^2}{4\mu}} \left[ A + \frac{B}{2\mu} \vec{\sigma} \cdot \vec{q} \right]
\]
\[
= \left( \frac{\pi}{\mu} \right)^{3/2} e^{-\frac{\vec{q}^2}{4\mu}} \left[ A + \frac{iB}{2\mu} [q_+ \hat{\sigma}_- + q_- \hat{\sigma}_+ + q_z \hat{\sigma}_z] \right]
\]
where
\[
q_\pm = q_x \pm iq_y \quad \text{and} \quad \sigma_\pm = \frac{1}{2} (\sigma_x \pm i\sigma_y)
\]

Since the initial spin is oriented along \( \hat{k} \), which we choose to be in the \( z \)-direction, we also quantize the final spin along the same axis (use the same representation).

How do the different terms scatter spins?

1. The term \( A \) is spin-independent. This implies that the final spin state is the same as the initial spin state and the value of this term is \( A \).

2. The term \( Bq_z \hat{\sigma}_z \) is a diagonal operator in this representation. This implies that the final spin state is the same as the initial spin state and the value of this term is \( Bq_z \). We only get the plus sign because we assumed spin up in the initial state.

3. The term \( Bq_+ \hat{\sigma}_- \) flips the spin from \( +z \) to \( -z \). This implies the value is \( Bq_+ \) in a final state with the spin flipped (lowered).

4. The term \( Bq_- \hat{\sigma}_+ \) gives a zero contribution since the initial spin cannot be raised.

Therefore, if the final state is \(|+z\rangle\) we get a contribution
\[
A + \frac{i}{2\mu} Bq_z
\]
and if the final state is \(|-z\rangle\) we get a contribution
\[
\frac{i}{2\mu} B(q_x + iq_y)
\]

To get the total contribution to \( f(\theta) \) we must square each separate term (these are not indistinguishable processes) and then sum over the final states. We get
\[
\left| A + \frac{i}{2\mu} Bq_z \right|^2 + \left| \frac{i}{2\mu} B(q_x + iq_y) \right|^2 = A^2 + \frac{B^2 q_z^2}{4\mu^2}
\]
Therefore, the differential cross section is

\[ \frac{d\sigma}{d\Omega} = \frac{\pi}{4\hbar v_\mu^3} \int \frac{k'}{k'}^2 dk' e^{-\frac{(\vec{k} - \vec{k}')^2}{2\mu}} \left( \frac{\hbar^2}{2m} \left( k^2 - k'^2 \right) \right) \left[ A^2 + \frac{B^2 (\vec{k} - \vec{k}')^2}{4\mu^2} \right] \]

\[ = \frac{\pi^2 m^2}{4\hbar^4 \mu^3} e^{-k^2(1 - \cos \theta)/2\mu} \left[ A^2 + \frac{B^2 k^2 (1 - \cos \theta)}{2\mu^2} \right] \]

13.3.20 Born approximation - Atomic Potential

Use the Born approximation to determine the differential cross section for the atomic potential seen by an incoming electron, which can be represented by the function

\[ V(r) = -Ze^2 \int \frac{\rho_T(\vec{r}') d^3\vec{r}'}{|\vec{r} - \vec{r}'|} \]

where

\[ \rho_T(\vec{r}') = \rho_{\text{nuclear}}(\vec{r}') + \rho_{\text{electronic}}(\vec{r}') = \delta(\vec{r}') - \rho(\vec{r}') \]

The atomic potential seen by an incoming electron can be represented by the function

\[ V(r) = -Ze^2 \int \frac{\rho_T(\vec{r}') d^3\vec{r}'}{|\vec{r} - \vec{r}'|} \]

where

\[ \rho_T(\vec{r}') = \rho_{\text{nuclear}}(\vec{r}') + \rho_{\text{electronic}}(\vec{r}') = \delta(\vec{r}') - \rho(\vec{r}') \]

We then have

\[ f(\theta) = \frac{mZe^2}{2\pi \hbar^2} \int \frac{\rho_T(\vec{r}') e^{i\vec{q} \cdot \vec{r}'} d^3\vec{r}'}{|\vec{r} - \vec{r}'|} d^3\vec{r}' \]

\[ = \frac{mZe^2}{2\pi \hbar^2} \int \rho_T(\vec{r}') e^{i\vec{q} \cdot \vec{r}'} d^3\vec{r}' \int \frac{e^{i\vec{q} \cdot (\vec{r} - \vec{r}')}}{|\vec{r} - \vec{r}'|} d^3\vec{r} \]
In the last integral $\vec{r}'$ is a constant. Therefore we can write

$$\int \frac{e^{i\vec{q}\cdot (\vec{r} - \vec{r}')}}{|\vec{r} - \vec{r}'|} d^3\vec{r}' = \int \frac{e^{i\vec{q}\cdot \vec{r}}}{x} d^3\vec{x}$$

$$= \lim_{\alpha \to 0} \int d\varphi \int_0^\pi \sin \theta d\theta \int_0^\infty e^{-\alpha x} e^{iqx \cos \theta} x dx$$

$$= 2\pi \lim_{\alpha \to 0} \int_0^\infty e^{-\alpha x} x dx \int_0^\pi \sin \theta d\theta e^{iqx \cos \theta}$$

$$= 2\pi \lim_{\alpha \to 0} \int_0^\infty e^{-\alpha x} x dx \left[ \frac{e^{iqx} - e^{-iqx}}{iqx} \right]$$

$$= \frac{4\pi}{q} \lim_{\alpha \to 0} \int_0^\infty e^{-\alpha x} \sin qx dx$$

$$= \frac{4\pi}{q} \lim_{\alpha \to 0} \frac{q}{q^2 + \alpha^2} = \frac{4\pi}{q^2}$$

This trick of introducing the integrating factor $e^{-ax}$ is a very useful procedure for evaluating this type of integral. We then have

$$f(\theta) = \frac{2mZe^2}{\hbar^2 q^2} \int \rho_T(\vec{r}') e^{i\vec{q}\cdot \vec{r}'} d^3\vec{r}'$$

$$= \frac{2mZe^2}{\hbar^2 q^2} \left[ \rho(\vec{r}') - \rho(\vec{r}') \right] e^{i\vec{q}\cdot \vec{r}'} d^3\vec{r}'$$

$$= \frac{2mZe^2}{\hbar^2 q^2} [1 - F(q)]$$

where

$$F(q) = \int \rho(\vec{r}') e^{i\vec{q}\cdot \vec{r}'} d^3\vec{r}'$$

= the atomic scattering function energy of the nuclei

It is a measure of the amount of shielding of the nuclear charge by the electrons in the atom. It is the Fourier transform of the electron charge density.

### 13.3.21 Lennard-Jones Potential

Consider the Lennard-Jones potential (shown below) used to model the binding of two atoms into a molecule.
Figure 13.4: 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 $\hat{H}_0 = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$ and $\hat{H}_1 = \xi x^3$.

In the Lennard-Jones potential the first term corresponds to a short-range repulsion and the second term corresponds to a long-range attraction.

The equilibrium point $r_0$ is given by:

$$\left. \frac{dV}{dr} \right|_{r_0} = 0 = -\frac{12C_{12}}{r_0^{13}} + \frac{6C_6}{r_0^7} \rightarrow r_0 = \left( \frac{2C_{12}}{C_6} \right)^{1/6}$$

Now expanding in a Taylor series we have

$$V(r) = V(r_0) + \left. \frac{dV}{dr} \right|_{r_0} (r - r_0) + \frac{1}{2} \left. \frac{d^2V}{dr^2} \right|_{r_0} (r - r_0)^2 + \frac{1}{3!} \left. \frac{d^3V}{dr^3} \right|_{r_0} (r - r_0)^3 + \ldots$$

$$V_0 + \frac{1}{2} V_0'' (r - r_0)^2 + \frac{1}{6} V_0''' (r - r_0)^3 + \ldots$$

$$= V_0 + \frac{1}{2} m \omega^2 (r - r_0)^2 + \xi (r - r_0)^3 +$$

$$V_0 + \frac{1}{2} m \omega^2 x^2 + \xi x^3 + \ldots$$

where

$$m \omega^2 = V_0''', \quad \xi = \frac{1}{6} V_0'''' , \quad x = r - r_0$$
Therefore,

\[ H = \hat{H}_0 + \hat{H}_1 \]

where

\[ \hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2, \quad \hat{H}_1 = \xi \hat{x}^3 \]

(b) What is the small parameter of the perturbation expansion?

To find the small parameter, we seek the characteristic scales.

For \( \hat{H}_0 \to E_0 = \hbar \omega \) and for \( \hat{H}_1 \to E_1 = \xi x_0^3 \) where \( x_0 = \text{sqrth}/m \omega = \) characteristic width of wave packet. Therefore, we have as a small parameter

\[ \epsilon = \frac{E_1}{E_0} = \frac{\xi x_0^3}{\hbar \omega} \]

Alternatively, we could write this small parameter as

\[ \epsilon = \frac{\xi x_0^3}{\frac{1}{2} m \omega^2 x_0^2} = \frac{1}{6} \frac{V'''(r_0)}{V''(r_0)} x_0 \]

(c) Show that the first energy shift vanishes (use symmetry).

The zero-order eigenstates \( |n\rangle \), \( E_n = \hbar \omega (n + 1/2) \) give the first-order shift

\[ E^{(1)}_n = \langle n | \hat{H}_1 | n \rangle = \xi \int_{-\infty}^{\infty} dx |\phi_n(x)|^2 x^3 \]

Now the wave functions \( \phi_n(x) \) are eigenstates of parity so that \( |\phi_n(x)|^2 \) is an even function. However, \( x^3 \) is an odd function. Therefore, \( E^{(1)}_n = 0 \) for all \( n \).

(d) Show that the second energy shift (first nonvanishing correction) is

\[ E^{(2)}_n = \xi^2 \frac{\hbar^3}{3 \hbar \omega^2} \sum_{m \neq n} \left| \frac{\langle m | (\hat{\alpha} + \hat{\alpha}^+)^3 | n \rangle^2}{n - m} \right| \]

The second-order shift is

\[ E^{(2)}_n = \sum_{m \neq n} \frac{|\langle m | \hat{H}_1 | n \rangle|^2}{E^{(0)}_n - E^{(0)}_m} = \xi^2 \frac{\hbar^2}{\hbar \omega} \sum_{m \neq n} \frac{|\langle m | \hat{x}^3 | n \rangle|^2}{n - m} \]

Now

\[ \hat{x} = \frac{x_0}{\sqrt{2}} (\hat{\alpha} + \hat{\alpha}^+) \to |\langle m | \hat{x}^3 | n \rangle|^2 = \left( \frac{\hbar}{2m \omega} \right)^3 |\langle m | (\hat{\alpha} + \hat{\alpha}^+)^3 | n \rangle|^2 \]
Therefore,

\[ E_n^{(2)} = \frac{\xi^2}{\hbar \omega} \sum_{m \neq n} \left| \langle m | (\hat{a} + \hat{a}^+)^3 | n \rangle \right|^2 \]

(c) Evaluate the matrix elements to show that

\[ E_n^{(2)} = \frac{\xi^2 \hbar^2}{m^3 \omega^4} \left[ \frac{(n-2)(n-1)(n)}{3} + \frac{(n+3)(n+2)(n+1)}{-3} + \frac{9n^3}{1} + \frac{9(n+1)^3}{-1} \right] \]

\[ = - \frac{\xi^2 \hbar^2}{m^3 \omega^4} \left[ \frac{15}{4} \left( n + 1/2 \right)^2 + \frac{7}{16} \right] \]

Using

\[ \hat{a} | n \rangle = \sqrt{n} | n - 1 \rangle, \quad \hat{a}^+ | n \rangle = \sqrt{n+1} | n + 1 \rangle \]

\[ \langle n | \hat{a} = \sqrt{n+1} \langle n + 1 |, \quad \langle n | \hat{a}^+ = \sqrt{n} \langle n - 1 | \]

\[ \langle n | m \rangle = \delta_{n,m}, \quad \hat{N} = \hat{a}^+ \hat{a} \]

we have

\[ (\hat{a} + \hat{a}^+)^3 = (\hat{a} + \hat{a}^+)(\hat{a}^2 + \hat{a}^{+2} + 2\hat{N} + 1) \]

\[ = \hat{a}^3 + \hat{a}^{+3} + \hat{a}^+ \hat{a}^2 + \hat{a} \hat{a}^{+2} + (\hat{a} + \hat{a}^+)(2\hat{N} + 1) \]

After using [\hat{a}, \hat{a}^+] = 1 we get

\[ (\hat{a} + \hat{a}^+)^3 = \hat{a}^3 + \hat{a}^{+3} + (3\hat{N} + 3)\hat{a} + 3\hat{N}\hat{a}^+ \]

Therefore,

\[ \langle m | \hat{a}^3 | n \rangle = \sqrt{n(n-1)(n-2)} \delta_{m,n-3} \]

\[ \langle m | \hat{a}^{+3} | n \rangle = \sqrt{(n+1)(n+2)(n+3)} \delta_{m,n+3} \]

\[ \langle m | (3\hat{N} + 3)\hat{a} | n \rangle = (3m + 3) \sqrt{n} \delta_{m,n-1} \]

\[ \langle m | 3\hat{N}\hat{a}^+ | n \rangle = 3m \delta_{m,n+1} \]

and therefore

\[ E_n^{(2)} = \frac{\xi^2 \hbar^2}{m^3 \omega^4} \left[ \frac{(n-2)(n-1)(n)}{3} + \frac{(n+3)(n+2)(n+1)}{-3} + \frac{9n^3}{1} + \frac{9(n+1)^3}{-1} \right] \]

\[ = - \frac{\xi^2 \hbar^2}{m^3 \omega^4} \left[ \frac{15}{4} \left( n + 1/2 \right)^2 + \frac{7}{16} \right] \]

(f) Consider carbon C-C bonds take Lennard-Jones parameters \( C_6 = 15.2 \text{ eV } \AA^6 \)

and \( C_{12} = 2.4 \times 10^4 \text{ eV } \AA^{12} \). Plot the potential and the energy levels from the ground to second excited state including the anharmonic shifts.

Therefore the equilibrium point is

\[ r_0 = \left( 2C_{12}/C_6 \right)^{1/6} = 3.8 \AA, \quad \epsilon = 0.35 \]

This implies that perturbation theory is fair (not great). This can be seen by the fact that \( \hbar \omega \) is on the order of the binding energy.
i.e., only two bound states.

**13.3.22 Covalent Bonds - Diatomic Hydrogen**

Consider the simplest neutral molecule, diatomic hydrogen $H_2$, consisting of two electrons and two protons.

![Figure 13.5: Diatomic Molecule](image)

(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)?

Classically, in order to bond two protons together, one must have the maximum negative charge between them.

Of course, this is not a stable configuration. Classically, one cannot bound a molecule solely with classical electrostatic forces.

The maximum repulsion occurs when the two electrons are as far apart as possible.
(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?

We consider a diatomic Hydrogen molecule. The nuclei move in the presence of the electron density associated with fixed orbitals (the Born-Oppenheimer approximation). We approximate these as products of atomic orbitals, properly symmetrized. Thus we have

$$ |\psi_{12} \rangle = \frac{1}{\sqrt{2}} (|\phi_A\rangle_1 |\phi_B\rangle_2 \pm |\phi_B\rangle_1 |\phi_A\rangle_2) \otimes |\chi\rangle $$

where

$$ |\phi_A\rangle \rightarrow \phi_{1s}(\vec{r} + \vec{R}/2) = 1s \text{ orbital centered at nucleus A} $$

$$ |\phi_B\rangle \rightarrow \phi_{1s}(\vec{r} - \vec{R}/2) = 1s \text{ orbital centered at nucleus B} $$

and

$$ |\chi\rangle = \text{Spin state} = \begin{cases} \text{singlet} & \rightarrow \text{symmetric space function} \\ \text{triplet} & \rightarrow \text{antisymmetric space function} \end{cases} $$

The joint probability density for the two electrons to be halfway between the two nuclei (at the origin) is

$$ |\psi_{12}(\vec{r}_1 = 0, \vec{r}_2 = 0)|^2 = |\phi_A(0)|^2 |\phi_B(0)|^2 \pm |\phi_A(0)|^2 |\phi_B(0)|^2 $$

These two terms are called the direct and exchange terms, respectively.

The singlet gives constructive interference- the electrons bunch together at origin - this is the bonding configuration.

The triplet gives destructive interference- the electrons maximally anti-bonded - this is the anti-bonding configuration.

(c) Sketch the potential energy seen by the nuclei as a function of the internuclear separation $R$ for the two different electron configurations. Your bonding configuration should allow for bound-states of the nuclei to one another. This is the covalent bond.

For small $R$ we have a repulsive Coulomb potential $e^2/R$.

For $R \rightarrow \infty$ we have two independent atoms with no interaction.

For large but not infinite $R$, we have two configurations:

- singlet which has lower energy
- triplet which has higher energy
The potential energy looks like:

![Potential Energy Diagram]

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).

We first need to determine the potential for the electron cloud. Assuming a uniform sphere of charge, the electric field is easily seen to be

$$E(r) = \begin{cases} \frac{-e}{a_0} & r < a_0 \\ \frac{-e}{r} & r \geq a_0 \end{cases}$$

(i.e., it grows linearly inside the sphere, but falls off as an inverse square law outside the sphere). Integrating to find the electric potential,

$$\phi(r) = -\int_{\infty}^{r} E(r')dr'$$

we find

$$\phi(r) = \begin{cases} -\frac{e}{a_0} \left( \frac{1}{2} \left( \frac{r}{a_0} \right)^2 - \frac{3}{2} \right) & r < a_0 \\ -\frac{e}{r} & r \geq a_0 \end{cases}$$

To this, we have to add the electric potential from the proton, $e/r$. We see that the total potential vanishes outside of $a_0$ (since the hydrogen atom}
is neutral after all). For interaction with a particle of charge \( Q = Ne \), the potential energy (charge times electric potential) is then

\[
V(r) = \frac{Ne^2}{a_0} \left( \frac{1}{2} \left( \frac{r}{a_0} \right)^2 - \frac{3}{2} + \frac{a_0}{r} \right), \quad r < a_0 \text{ only}
\]

All we need to do now is to substitute this into the expression for the Born amplitude

\[
f_{\text{Born}}(\theta) = -\frac{2m}{\hbar^2} \int_0^\infty V(r) \frac{\sin qr}{qr} r^2 dr
\]

where

\[
q = 2k \sin \frac{\theta}{2}
\]

We perform a change of variable, \( x = qr \), to find

\[
f_{\text{Born}}(\theta) = \frac{2mNe^2}{\hbar^2 q^2 a_0^2} \int_0^{qa_0} \left( \frac{1}{2} \left( \frac{r}{a_0} \right)^2 - \frac{3}{2} + \frac{a_0}{r} \right) \frac{\sin qr}{qr} r^2 dr
\]

Now using

\[
\int \sin x \, dx = -\cos x
\]

\[
\int x \sin x \, dx = -x \cos x + \sin x
\]

\[
\int x^3 \sin x \, dx = -x(x^2 - 6) \cos x + 3(x^2 - 2) \sin x
\]

we find

\[
f_{\text{Born}}(\theta) = \frac{2mNe^2}{\hbar^2 q^2 a_0^2} \left( (qa_0)^2 + 3 \cos (qa_0) - \frac{3 \sin (qa_0)}{qa_0} \right)
\]

The differential cross section is thus

\[
d\sigma = |f_{\text{Born}}(\theta)|^2 = \frac{4m^2 N^2 e^4}{\hbar^4 q^3 a_0^4} \left( (qa_0)^2 + 3 \cos (qa_0) - \frac{3 \sin (qa_0)}{qa_0} \right)^2
\]

(b) What is the form of the differential cross section for low energy? Compare with the pure Coulomb cross section.

For low energies, \( qa_0 \ll 1 \), we may expand

\[
( (qa_0)^2 + 3 \cos (qa_0) - \frac{3 \sin (qa_0)}{qa_0} ) \approx \frac{1}{1} (qa_0)^4 + .......
\]

(note that the first two orders cancel in the Taylor expansion), to obtain

\[
d\sigma = \frac{m^2 N^2 e^4 a_0^4}{25\hbar^4} (qa_0 < 1)
\]

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This may be written more suggestively by using the expression for the Bohr radius, $a_0 = \frac{\hbar^2}{me^2}$ to obtain

$$\frac{d\sigma}{d\Omega} = \frac{N^2}{25}a_0^2$$

which has the form of a hard-sphere cross section (at low energies), with scattering $a = Na_0/5$. This is certainly not the pure Coulomb cross section. But there is no reason to expect it to be either. At low energies, we do not expect to probe inside the electron cloud, and the hydrogen atom looks essentially like a hard sphere. We can think of the Coulomb potential as being perfectly screened by the hydrogen electron at large distance scales (corresponding to low energies).

(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.

When the energy is raised, we need to consider the limit $qa_0 >> 1$. In this case, the expansion

$$\left((qa_0)^2 + 3 \cos(qa_0) - 3\frac{\sin(qa_0)}{qa_0}\right) \approx \frac{1}{1}(qa_0)^2 + \ldots$$

is straightforward. This gives

$$\frac{d\sigma}{d\Omega} = \frac{4m^2N^2e^4}{\hbar^4q^4}a_0^2 = \frac{m^2N^2e^4}{4(h\kappa)^4\sin^4\frac{\theta}{2}} \quad (qa_0 >> 1)$$

which is just the Rutherford formula for Coulomb scattering. At high energies, we can probe at smaller distances (given by the Compton wavelength). So in this case we can penetrate the electron cloud and see the bare (unscreened) Coulomb potential of the proton. This is why the limiting case looks more and more like Coulomb scattering.
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 $\hat{n} = \cos \theta \hat{\sigma}_z - \sin \theta \hat{\sigma}_x$ (see figure below).

![Figure 15.1: Tilted Stern-Gerlach Setup](image)

What is the probability of finding the outgoing particle in the state?

The eigenvalue relation

$$(\hat{n} \cdot \vec{S}) |S_n\pm\rangle = \pm \frac{\hbar}{2} |S_n\pm\rangle$$

where

$$\hat{n} \cdot \vec{S} = \cos \theta \hat{\sigma}_z - \sin \theta \hat{\sigma}_x = \cos \theta \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \sin \theta \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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is represented in matrix form as
\[
\begin{pmatrix}
\cos \theta & -\sin \theta \\
-\sin \theta & -\cos \theta
\end{pmatrix}
\begin{pmatrix}
a \\
b
\end{pmatrix}
= \pm
\begin{pmatrix}
a \\
b
\end{pmatrix}
\]
Solving, we obtain \(a_+ = \cos \left( \frac{\theta}{2} \right) = b_-\) and \(a_- = \sin \left( \frac{\theta}{2} \right) = -b_+\). This gives
\[
|S_n^+\rangle = \left( \cos \left( \frac{\theta}{2} \right) \right), \quad |S_n^-\rangle = \left( \sin \left( \frac{\theta}{2} \right) \right)
\]
The probability of finding the particle in the state \(|S_n^+\rangle\) is
\[
P = |\langle S_n^+ | S_z^+ \rangle|^2 = \cos^2 \left( \frac{\theta}{2} \right)
\]
(b) Now consider a Stern-Gerlach device of variable orientation as in the figure below.

![Figure 15.2: Variable Orientation Stern-Gerlach Setup](image)

More specifically, assume that it can have the three different directions
\[
\hat{n}_1 = \hat{n} = \cos \theta \hat{z} - \sin \theta \hat{x} \\
\hat{n}_2 = \cos \left( \theta + \frac{2\pi}{3} \right) \hat{z} - \sin \left( \theta + \frac{2\pi}{3} \right) \hat{x} \\
\hat{n}_3 = \cos \left( \theta + \frac{4\pi}{3} \right) \hat{z} - \sin \left( \theta + \frac{4\pi}{3} \right) \hat{x}
\]
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 \(+\hbar/2\)?

The probability of finding a particle in the exit beam carrying spin eigenvalue \(+\hbar/2\) is
\[
P = \frac{1}{3} \sum_{i=1}^{3} |\langle S_{n_i}^+ | S_z^+ \rangle|^2 \\
= \frac{1}{3} \left( \cos^2 \left( \frac{\theta}{2} \right) + \cos^2 \left( \frac{\theta}{2} + \frac{\pi}{3} \right) + \cos^2 \left( \frac{\theta}{2} + \frac{2\pi}{3} \right) \right)
\]
Using
\[
\cos\left(\frac{\theta}{2} + \frac{\pi}{3}\right) = \frac{1}{2} \cos\left(\frac{\theta}{2}\right) - \frac{\sqrt{3}}{2} \sin\left(\frac{\theta}{2}\right)
\]
\[
\cos\left(\frac{\theta}{2} + \frac{2\pi}{3}\right) = -\cos\left(\frac{\theta - \pi}{3}\right) = -\frac{1}{2} \cos\left(\frac{\theta}{2}\right) - \frac{\sqrt{3}}{2} \sin\left(\frac{\theta}{2}\right)
\]
this can be seen to give
\[
P = \frac{1}{3} \cos^2\left(\frac{\theta}{2}\right) + \frac{1}{2} \cos^2\left(\frac{\theta}{2}\right) + \frac{3}{2} \sin^2\left(\frac{\theta}{2}\right) = \frac{1}{2}
\]

(c) Calculate the same probability as above but now for a Stern-Gerlach analyzer that can have any orientation with equal probability.

In this case we should average over all the orientations according to
\[
\langle....\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta....
\]
Then we have
\[
P = \langle|\langle S_n^+|S_z^+\rangle|^2\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \cos^2\left(\frac{\theta}{2}\right) = \frac{1}{2}
\]

(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](image)

The probability of opposite spin outcomes is
\[
P = \left\langle\left[\langle 0,0|S_n^{(1)}+\rangle\right|\left|S_{n'}^{(2)}-\right\rangle\right|^2 + \left\langle\langle 0,0|S_n^{(1)}-\rangle\right|\left|S_{n'}^{(2)}+\right\rangle\right|^2\right\rangle
\]
\[
= \left\langle\cos^4\frac{\theta - \theta'}{2}\right\rangle = \frac{1}{2}
\]

The intermediate steps involved are:
\[
\langle + | \hat{n}^-\rangle \langle - | \hat{n}^+\rangle - \langle - | \hat{n}^+\rangle \langle + | \hat{n}^-\rangle = \cos \frac{1}{2} (\theta - \theta')
\]
\[
\langle + | \hat{n}^-\rangle \langle - | \hat{n}^+\rangle - \langle - | \hat{n}^-\rangle \langle + | \hat{n}^+\rangle = -\cos \frac{1}{2} (\theta - \theta')
\]

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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 \( a \to 0 \).

The normalization constant is

\[ N = \sqrt{\frac{2}{\pi}} (\alpha\beta)^{-1/4} \]

In the limit \( \alpha \to 0 \)

\[ \psi(x_1, x_2) \sim \frac{1}{\pi} \delta(x_1 - x_2 + a) \left( \frac{\alpha}{\beta} \right)^{1/4} \exp \left[ -\frac{1}{2\beta} (x_1 + x_2)^2 \right] \]

This is a sharply localized amplitude describing the situation where the two particles are at a distance \( x_2 - x_1 = a \). Keeping \( \alpha \) as small as we wish but non-zero and \( \beta \) as large as we wish but not infinite, we have a normalizable amplitude for the two particles to be at distance \( a \), to any order of approximation.

(b) Calculate the momentum space wave function and discuss its properties in the above limit.

The momentum space wave function is

\[ \Phi(p_1, p_2) = \frac{(\alpha\beta)^{1/4}}{\sqrt{2\pi}} \exp \left[ \frac{i}{2} (p_1 - p_2)a - \frac{\alpha}{8} (p_1 - p_2)^2 - \frac{\beta}{8} (p_1 + p_2)^2 \right] \]

In the limit \( \beta \to \infty \) we have

\[ \Phi(p_1, p_2) \sim \delta(p_1 + p_2) 2 \left( \frac{\alpha}{\beta} \right)^{1/4} \exp \left[ \frac{i}{2} (p_1 - p_2)a \right] \exp \left[ -\frac{\alpha}{8} (p_1 - p_2)^2 \right] \]

This is a sharply localized momentum-space for the two particles to have opposite momenta. Keeping \( \beta \) as large as we wish but finite and \( \alpha \) as small as we wish, we have a normalizable amplitude for the two particles to have opposite momenta, to any desired order of approximation.

(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?

A measurement of \( x_1 \) and \( x_2 \) will yield values related by \( x_2 - x_1 = a \): the
measurement of the position of particle 1 is sufficient to determine the position of particle 2, or vice versa. A measurement of the momenta \( p_1 \) and \( p_2 \) will give values related by \( p_2 = -p_1 \): the measurement of the momentum of particle 2 is sufficient to determine the momentum of particle 1, or vice versa. This is an example of entanglement.

### 15.6.3 Measurements on a 2 Spin-1/2 System

(a) Consider a system of two spin-1/2 particles in the singlet state

\[
|1,0\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_{(1)} |\downarrow\rangle_{(2)} - |\downarrow\rangle_{(1)} |\uparrow\rangle_{(2)} \right)
\]

and perform a measurement of \( S_z^{(1)} \). Comment on the fact that a simultaneous measurement of \( S_z^{(2)} \) gives an outcome that can always be predicted from the first-mentioned measurement. Show that this property, entanglement, is not shared by states that are tensor products. Is this state \( |\psi\rangle = \frac{1}{2} \left( |\uparrow\rangle_{(1)} + \sqrt{2} |1,0\rangle + |1,-1\rangle \right) \) entangled, i.e., is it a tensor product?

A measurement of \( S_z^{(1)} \) when the system is in the state \( \text{Ket}1,0 \) will give \( \pm \hbar/2 \) with equal probability. If the value \( +\hbar/2 \) occurs, implying that particle 1 is in the state \( |\uparrow\rangle \), a measurement of \( S_z^{(2)} \) will yield the value \( -\hbar/2 \), particle 2 being necessarily in the state \( |\downarrow\rangle \). Inversely, if a measurement on particle '1' projects it into the state \( |\downarrow\rangle \), a simultaneous measurement on the other particle will necessarily give \( +\hbar/2 \). The two particles are in an entangled state. In contrast, if the state of the two particles can be written as a tensor product then there is no entanglement. For the given state \( |\psi\rangle \), we have

\[
|\psi\rangle = \frac{1}{2} \left( (|\uparrow\rangle |\uparrow\rangle + |\downarrow\rangle |\downarrow\rangle + |\downarrow\rangle |\uparrow\rangle + |\uparrow\rangle |\downarrow\rangle \right)
\]

or

\[
|\psi\rangle = \left( \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle) \right) \otimes \left( \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle) \right)
\]

A spin measurement of particle 1 with outcome \( \pm \hbar/2 \) can be accompanied by a spin measurement of particle '2' with either of the outcomes \( \pm \hbar/2 \). The two particles are completely disentangled.
(b) Consider now the set of four states $|a\rangle$, $a = 0, 1, 2, 3$:

\begin{align*}
|0\rangle &= \frac{1}{\sqrt{2}} (|1,1\rangle + i |1,-1\rangle) \\
|1\rangle &= \frac{1}{\sqrt{2}} (|1,-1\rangle + i |1,1\rangle) \\
|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{align*}

Show that these states are entangled and find the unitary matrix $U_{a\alpha}$ such that

$$|a\rangle = U_{a\alpha} |\alpha\rangle$$

where $\{|\alpha\rangle\} = |1,1\rangle, |1,-1\rangle, |1,0\rangle, |0,0\rangle$.

The given states can be written in terms of the product states as

\begin{align*}
|0\rangle &= \frac{1}{\sqrt{2}} (|\uparrow\rangle |\uparrow\rangle + i |\downarrow\rangle |\downarrow\rangle) \\
|1\rangle &= \frac{1}{\sqrt{2}} (|\downarrow\rangle |\downarrow\rangle + i |\uparrow\rangle |\uparrow\rangle) \\
|2\rangle &= \frac{1}{\sqrt{2}} (|\downarrow\rangle |\uparrow\rangle - i |\uparrow\rangle |\downarrow\rangle) \\
|3\rangle &= \frac{1}{\sqrt{2}} (|\uparrow\rangle |\downarrow\rangle - i |\downarrow\rangle |\uparrow\rangle)
\end{align*}

A spin measurement of particle 1 in either of the first two states results in particle 2 having a spin of the same sign. Similarly, in each of the other two states a spin measurement of the first particle results in an antiparallel spin for the other.

The matrix $U$ is given by

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & i & 0 & 0 \\
0 & 0 & e^{-i\pi/4} & -e^{i\pi/4} \\
i & 1 & 0 & 0 \\
0 & 0 & e^{i\pi/4} & e^{-i\pi/4}
\end{pmatrix}$$

and it is straightforward to see that it is unitary.

(c) Consider a one-particle state $|\psi\rangle = C_+ |\uparrow\rangle + C_- |\downarrow\rangle$ and one of the entangled states considered in (b), for example $|0\rangle$. Show that the product state can be written as

$$|\psi\rangle |0\rangle = \frac{1}{2} (|0\rangle |\psi\rangle + |1\rangle |\psi'\rangle + |2\rangle |\psi''\rangle + |3\rangle |\psi'''\rangle)$$
where the states $|\psi\rangle$, $|\psi'\rangle$, $|\psi''\rangle$, are related to $|\psi\rangle$ through a unitary transformation.

Setting

$$|\psi'\rangle = D_+ |\uparrow\rangle + D_- |\downarrow\rangle$$
$$|\psi''\rangle = E_+ |\uparrow\rangle + E_- |\downarrow\rangle$$
$$|\psi'''\rangle = F_+ |\uparrow\rangle + F_- |\downarrow\rangle$$

and substituting into the expression to be proved, we obtain

$$\frac{1}{2} (|0\rangle |\psi\rangle + |1\rangle |\psi'\rangle + |2\rangle |\psi''\rangle + |3\rangle |\psi'''\rangle)$$

Comparing with

$$|\psi\rangle |0\rangle = \frac{1}{\sqrt{2}} (C_+ |\uparrow\rangle |\uparrow\rangle + i C_- |\downarrow\rangle |\downarrow\rangle + C_- |\downarrow\rangle |\uparrow\rangle + i C_+ |\uparrow\rangle |\downarrow\rangle)$$

we get

$$D_+ = -i C_+ , \ D_- = i C_- , \ E_+ = C_- , \ E_- = -C_+ , \ F_+ = i C_- , \ F_- = i C_+$$

and

$$|\psi'\rangle = -i C_+ |\uparrow\rangle + i C_- |\downarrow\rangle = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} |\psi\rangle$$
$$|\psi''\rangle = C_- |\uparrow\rangle - C_+ |\downarrow\rangle = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} |\psi\rangle$$
$$|\psi'''\rangle = i C_- |\uparrow\rangle + i C_+ |\downarrow\rangle = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} |\psi\rangle$$

According to the above, a system consisting of a spin–1/2 particle in a state $|\psi\rangle$ and a pair of spin–1/2 particles in any of the entangled states $|a\rangle$ will produce, if subject to a measurement on the latter, a particle in one of the states $|\psi\rangle$, $|\psi'\rangle$, $|\psi''\rangle$, $|\psi'''\rangle$. A complete teleportation of, say, state $|\psi\rangle$ would be achieved if we were to transfer classically the information contained in the specification of the unitary matrix.

### 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:
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 $\varphi$ is

$$P_{D_A} = \frac{1}{2} (\cos(\varphi/2) + \sin(\varphi/2))^2 = \frac{1}{2} (1 + \sin \varphi)$$

Repeat for the state $|\downarrow_z\rangle$ and show that

$$P_{D_A} = \frac{1}{2} (\cos(\varphi/2) - \sin(\varphi/2))^2 = \frac{1}{2} (1 - \sin \varphi)$$

In the setup above, the effect of the solenoid is to rotate the spin according to the Hamiltonian

$$\hat{H} = \frac{\mu_B B}{\hbar} \hat{\sigma}_y$$

so that the rotation operator is given by

$$\hat{R}_y = e^{-i\hat{H}t/\hbar} = e^{-i\Omega t \hat{\sigma}_y} e^{-i\varphi \hat{\sigma}_y}$$

$$\Omega = \frac{2\mu_B B}{\hbar}, \quad \Omega t = \varphi$$

so that

$$\hat{R}_y = \cos \frac{\varphi}{2} \hat{I} - i \sin \frac{\varphi}{2} \hat{\sigma}_y = \begin{pmatrix} \cos \frac{\varphi}{2} & -\sin \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} & \cos \frac{\varphi}{2} \end{pmatrix}$$

in the standard basis.

We have the initial state

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

Now,

$$\hat{R}_y |\uparrow_z\rangle = \begin{pmatrix} \cos \frac{\varphi}{2} & -\sin \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} & \cos \frac{\varphi}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} \end{pmatrix}$$

and thus

$$P(D_A) = |\langle \uparrow_z \mid \hat{R}_y \mid \uparrow_z \rangle|^2 = \left| \begin{pmatrix} 1 \sqrt{2} \\ 1 \sqrt{2} \end{pmatrix} \begin{pmatrix} \cos \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} \end{pmatrix} \right|^2 = \left( \cos \frac{\varphi}{2} + \sin \frac{\varphi}{2} \right)^2 = \frac{1}{2} (1 + \sin \varphi)$$
Now the initial state is
\[
|\downarrow_z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}
\]

Therefore,
\[
\hat{R}_y |\downarrow_z\rangle = \begin{pmatrix} \cos \frac{\varphi}{2} & -\sin \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} & \cos \frac{\varphi}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\sin \frac{\varphi}{2} \\ \cos \frac{\varphi}{2} \end{pmatrix}
\]

and thus,
\[
P(D_A) = \left| \langle \uparrow_x | \hat{R}_y |\downarrow_z\rangle \right|^2 = \left| (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})( -\sin \frac{\varphi}{2} \cos \frac{\varphi}{2} ) \right|^2 = \frac{(\cos \frac{\varphi}{2} - \sin \frac{\varphi}{2})^2}{2} = \frac{1}{2}(1-\sin \varphi)
\]

A plot of these results looks like:

(b) Now suppose the input is a pure coherent superposition of these two states,
\[
|\uparrow_x\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle + |\downarrow_z\rangle)
\]

Find and sketch the probability for detector $D_A$ to fire as a function of $\varphi$.

We now consider the initial state
\[
|\uparrow_x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\]

Now
\[
\hat{R}_y |\uparrow_x\rangle = \begin{pmatrix} \cos \frac{\varphi}{2} & -\sin \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} & \cos \frac{\varphi}{2} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos \frac{\varphi}{2} - \sin \frac{\varphi}{2} \\ \cos \frac{\varphi}{2} + \sin \frac{\varphi}{2} \end{pmatrix}
\]

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and thus
\[ P(D_A) = \left| \langle \uparrow_x | \hat{R}_y | \uparrow_x \rangle \right|^2 = \left| \left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right) \left( \frac{\cos \frac{\phi}{2} - \sin \frac{\phi}{2}}{\sqrt{2}} \right) \right|^2 = \cos^2 \frac{\phi}{2} \]

A plot of these results looks like:

(c) Now suppose the input state is the completely mixed state
\[ \hat{\rho} = \frac{1}{2} (|\uparrow_z \rangle \langle \uparrow_z | + |\downarrow_z \rangle \langle \downarrow_z |) \]
Find and sketch the probability for detector \( D_A \) to fire as a function of \( \varphi \). Comment on the result.

We now consider the initial state
\[ \hat{\rho} = \frac{1}{2} (|\uparrow_z \rangle \langle \uparrow_z | + |\downarrow_z \rangle \langle \downarrow_z |) \]

In this case we have
\[ P(D_A) = \frac{1}{2} P(\uparrow_x | \uparrow_z) + \frac{1}{2} P(\uparrow_x | \downarrow_z) = \frac{1}{2} \left( \frac{1}{2}(1 + \sin \varphi) + \frac{1}{2}(1 - \sin \varphi) \right) = \frac{1}{2} \]
for all \( \varphi \). A plot of these results looks like:
15.6.5 Mixed States vs. Pure States and Interference

A spin-interferometer is shown below:

Figure 15.5: Spin-Interferometer Setup

Spin−1/2 electrons prepared in a given state (pure or mixed) are separated into two paths by a Stern-Gerlach apparatus (gradient field along \( z \)). In one path, 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 \( \varphi \), 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 \( \varphi \) for the following pure state inputs:

\[
(i) \ |\uparrow_z\rangle, \quad (ii) \ |\downarrow_z\rangle, \quad (iii) \ |\uparrow_x\rangle, \quad (iv) \ |\downarrow_x\rangle
\]

Comment on your results.

Given the setup above, consider the pure state

\[
|\psi\rangle = C_\uparrow |\uparrow_z\rangle + C_\downarrow |\downarrow_z\rangle
\]
The spin state $|\uparrow_z\rangle$ branch gets rotated by the operator
$$\hat{R}_x(\varphi) = e^{-i\varphi \hat{\sigma}_x/2} = \cos\left(\frac{\varphi}{2}\right) - i\hat{\sigma}_x \sin\left(\frac{\varphi}{2}\right)$$
This implies that right before the final beam splitter we have the state
$$|\psi'\rangle = C_\uparrow \hat{R}_x(\varphi) |\uparrow_z\rangle + C_\downarrow |\downarrow_z\rangle$$
so that the probability of detector $D_A$ firing is
$$P_{D_A} = |\langle \uparrow_x | \psi' \rangle|^2 = |C_\uparrow \langle \uparrow_x | \hat{R}_x(\varphi) |\uparrow_z\rangle + C_\downarrow \langle \uparrow_x | \downarrow_z\rangle|^2$$

**ASIDE:**
$$\langle \uparrow_x | \hat{R}_x(\varphi) |\uparrow_z\rangle = \cos\left(\frac{\varphi}{2}\right) \langle \uparrow_x | \uparrow_z\rangle - i \sin\left(\frac{\varphi}{2}\right) \langle \uparrow_x | \hat{\sigma}_x |\uparrow_z\rangle$$

Now,
$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle + |\downarrow_z\rangle) \Rightarrow \langle \uparrow_x | \uparrow_z\rangle = \frac{1}{\sqrt{2}}, \quad \langle \uparrow_x | \hat{\sigma}_x |\uparrow_z\rangle = \langle \uparrow_x | \uparrow_z\rangle = \frac{1}{\sqrt{2}}$$
so that
$$P_{D_A} = |\langle \uparrow_x | \psi' \rangle|^2 = \frac{1}{2} \left| C_\uparrow \left( \cos\left(\frac{\varphi}{2}\right) - i \sin\left(\frac{\varphi}{2}\right) \right) + C_\downarrow \right|^2 = \frac{1}{2} \left| C_\uparrow e^{-i\varphi/2} + C_\downarrow \right|^2$$
$$= \frac{1}{2} \left( |C_\uparrow|^2 + |C_\downarrow|^2 + 2 \text{Re}(C_\uparrow C_\downarrow e^{-i\varphi/2}) \right)$$

(i) $|\psi\rangle = |\uparrow_z\rangle \Rightarrow C_\uparrow = 1, \ C_\downarrow = 0 \Rightarrow P_{D_A} = 1/2 = \text{constant}$. This case shows no interference because we know which path.

(ii) $|\psi\rangle = |\downarrow_z\rangle \Rightarrow C_\uparrow = 0, \ C_\downarrow = 1 \Rightarrow P_{D_A} = 1/2 = \text{constant}$. This case shows no interference because we know which path.

(iii) $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle + |\downarrow_z\rangle) \Rightarrow C_\uparrow = C_\downarrow = \frac{1}{\sqrt{2}} \Rightarrow P_{D_A} = \frac{1}{2} \left( \frac{1}{2} + \frac{1}{2} + \text{Re}(e^{-i\varphi/2}) \right) = \frac{1+\cos\frac{\varphi}{2}}{2} = \cos^2 \frac{\varphi}{2}$
This case shows interference fringes.

(iv) $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle - |\downarrow_z\rangle) \Rightarrow C_\uparrow = -C_\downarrow = \frac{1}{\sqrt{2}} \Rightarrow P_{D_A} = \frac{1}{2} \left( \frac{1}{2} + \frac{1}{2} - \text{Re}(e^{-i\varphi/2}) \right) = \frac{1-\cos\frac{\varphi}{2}}{2} = \sin^2 \frac{\varphi}{2}$
This case shows interference fringes.

(b) Remember that for a mixed state we have
$$\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle \psi_i|$$
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 \textit{classically}, i.e., we have one of the set \( \{ |\psi_i\rangle \} \), we just do not know which one.

Prove that

\[
P_{DA} = Tr \| \langle \uparrow_x | \hat{\rho} \rangle = \sum_i p_i |\langle \uparrow_x | \psi_i \rangle|^2
\]

where \( |\langle \uparrow_x | \psi_i \rangle|^2 \) = the probability of detector B firing for the given input state (we figured these out in part (a)). Repeat part (a) for the following mixed state inputs:

(i) \( \hat{\rho} = \frac{1}{2} |\uparrow_z\rangle \langle \uparrow_z| + \frac{1}{2} |\downarrow_z\rangle \langle \downarrow_z| \) ,
(ii) \( \hat{\rho} = \frac{1}{2} |\uparrow_x\rangle \langle \uparrow_x| + \frac{1}{2} |\downarrow_x\rangle \langle \downarrow_x| \) ,
(iii) \( \hat{\rho} = \frac{1}{3} |\uparrow_z\rangle \langle \uparrow_z| + \frac{2}{3} |\downarrow_z\rangle \langle \downarrow_z| \)

We now consider mixed states. Generally

\[
\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle \psi_i |
\]

This is a \textit{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. This implies that

\[
P_{DA} = Tr \| \langle \uparrow_x | \hat{\rho} \rangle = \sum_i \langle \psi_i | \langle \uparrow_x | \hat{\rho} | \psi_i \rangle
= \sum_i \langle \psi_i | \langle \uparrow_x | \sum_k p_k |\psi_k\rangle \langle \psi_k \rangle | \psi_i \rangle
= \sum_{i,k} p_k \langle \psi_i | \langle \uparrow_x | \psi_k \rangle \langle \psi_k | \psi_i \rangle
= \sum_{i,k} p_k \langle \psi_i | \langle \uparrow_x | \psi_k \rangle \delta_{ki} \sum_i p_i \langle \psi_i | \langle \uparrow_x | \psi_i \rangle = \sum_i p_i |\langle \uparrow_x | \psi_i \rangle|^2
\]

(i)

\[
\hat{\rho} = \frac{1}{2} |\uparrow_z\rangle \langle \uparrow_z| + \frac{1}{2} |\downarrow_z\rangle \langle \downarrow_z|

P_{DA} = \frac{1}{2} P_{DA}(\uparrow_z) + \frac{1}{2} P_{DA}(\downarrow_z) = \frac{1}{2} \frac{1}{2} + \frac{1}{2} \frac{1}{2} = \frac{1}{2}
\]

from part(a).

(ii)

\[
\hat{\rho} = \frac{1}{2} |\uparrow_x\rangle \langle \uparrow_x| + \frac{1}{2} |\downarrow_x\rangle \langle \downarrow_x|

P_{DA} = \frac{1}{2} P_{DA}(\uparrow_x) + \frac{1}{2} P_{DA}(\downarrow_x) = \frac{1}{2} \cos^2 \varphi + \frac{1}{2} \sin^2 \varphi = \frac{1}{2}
\]

from part(a).
Thus, we see that for a completely mixed state, the interference is removed.

\[ (iii) \]

\[
\hat{\rho} = \frac{1}{3} |\uparrow_z\rangle \langle \uparrow_z| + \frac{2}{3} |\downarrow_z\rangle \langle \downarrow_z|
\]

\[ P_{DA} = \frac{1}{3} P_{DA}(\uparrow_x) + \frac{2}{3} P_{DA}(\downarrow_x) = \frac{1}{3} \cos^2 \varphi + \frac{2}{3} \sin^2 \varphi = \frac{1}{3} + \frac{1}{3} \sin^2 \varphi \]

from part (a).

This represents interference fringes with reduced visibility (contrast). Thus a partial mixed state of two states which show interference shows fringes with reduced visibility.

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:

![Spin-Interferometer Setup](image)

**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 \(|\uparrow_z\rangle_W \rightarrow |\downarrow_z\rangle_W\), i.e, the "which-way" detector works such that

- If \(|\psi\rangle_D = |\uparrow_z\rangle_D\), nothing happens to \(|\uparrow_z\rangle_W\)
- If \(|\psi\rangle_D = |\downarrow_z\rangle_D\), then \(|\uparrow_z\rangle_W \rightarrow |\downarrow_z\rangle_W\) (a spin flip)

Thus, as a composite system

\[ |\uparrow_z\rangle_D |\uparrow_z\rangle_W \rightarrow |\uparrow_z\rangle_D |\uparrow_z\rangle_W \quad |\downarrow_z\rangle_D |\uparrow_z\rangle_W \rightarrow |\uparrow_z\rangle_D |\downarrow_z\rangle_W \]

(a) The electron D is initially prepared in the state \(|\uparrow_z\rangle_D = (|\uparrow_z\rangle_D + |\downarrow_z\rangle_D) / \sqrt{2}\). Show that before detection, the two electrons D and W are in an entangled state

\[ |\Psi_{DW}\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle_D |\uparrow_z\rangle_W + |\downarrow_z\rangle_D |\downarrow_z\rangle_W) \]
The "which-way" detector works such that

If \( |\psi\rangle_D = |\uparrow_z\rangle \) nothing happens to \(|\uparrow_w\rangle\)

If \( |\psi\rangle_D = |\downarrow_z\rangle \) then \(|\uparrow_w\rangle \rightarrow |\downarrow_w\rangle \) (a spin flip)

As a composite system

\[
\begin{align*}
|\uparrow_z\rangle_D |\uparrow_z\rangle_W & \rightarrow |\uparrow_z\rangle_D |\uparrow_z\rangle_W \\
|\downarrow_z\rangle_D |\uparrow_z\rangle_W & \rightarrow |\downarrow_z\rangle_D |\downarrow_z\rangle_W
\end{align*}
\]

Consider then a state of electron \( D \) which is in a superposition of up and down.

\[
|\uparrow_z\rangle_D = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle_D + |\downarrow_z\rangle_D)
\]

The composite system before \( D \) and \( W \) interact is

\[
|\uparrow_z\rangle_D |\uparrow_z\rangle_W = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle_D + |\downarrow_z\rangle_D) |\uparrow_z\rangle_W = \frac{1}{\sqrt{2}} |\uparrow_z\rangle_D |\uparrow_z\rangle_W + \frac{1}{\sqrt{2}} |\downarrow_z\rangle_D |\uparrow_z\rangle_W
\]

which after the interaction becomes

\[
\frac{1}{\sqrt{2}} |\uparrow_z\rangle_D |\uparrow_z\rangle_W + \frac{1}{\sqrt{2}} |\downarrow_z\rangle_D |\downarrow_z\rangle_W
\]

which is an entangled state.

(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

\[
\text{Prob}(m_D) = \sum_{m_W} |\langle m_D, m_W | \Psi_{DW} \rangle|^2
\]

for some observable.

This state shows no interference between \(|\uparrow_z\rangle_D \) and \(|\downarrow_z\rangle_D \). Thus, the which-way detector removes the coherence between states that existed in the input.

Given the state of the composite

\[
|\Psi_{DW} \rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle_D |\uparrow_z\rangle_W + |\downarrow_z\rangle_D |\downarrow_z\rangle_W)
\]
we ask - what is the state of $D$ alone? To answer this question, we consider the marginal probability distribution for some observable

$$P(m_D) = \frac{1}{2} \sum_{m_W} |\langle m_D | \uparrow_z \rangle_D \langle m_W | \uparrow_z \rangle_W|^2 + \frac{1}{2} |\langle m_D | \downarrow_z \rangle_D \langle m_W | \downarrow_z \rangle_W|^2$$

$$= \frac{1}{2} |\langle m_D | \uparrow_z \rangle_D|^2 \sum_{m_W} |\langle m_W | \uparrow_z \rangle_W|^2 + \frac{1}{2} |\langle m_D | \downarrow_z \rangle_D|^2 \sum_{m_W} |\langle m_W | \downarrow_z \rangle_W|^2$$

$$+ \frac{1}{2} \langle m_D | \downarrow_z \rangle_D^* \langle m_D | \uparrow_z \rangle_D \sum_{m_W} \langle m_W | \downarrow_z \rangle^*_W \langle m_W | \uparrow_z \rangle_W$$

$$+ \frac{1}{2} \langle m_D | \uparrow_z \rangle_D^* \langle m_D | \downarrow_z \rangle_D \sum_{m_W} \langle m_W | \uparrow_z \rangle^*_W \langle m_W | \downarrow_z \rangle_W$$

**ASIDE:**

$$\sum_{m_W} |\langle m_W | \uparrow_z \rangle_W|^2 = \sum_{m_W} |\langle m_W | \downarrow_z \rangle_W|^2 = 1$$

$$\sum_{m_W} \langle m_W | \downarrow_z \rangle^*_W \langle m_W | \uparrow_z \rangle_W = w \langle \downarrow_z | \uparrow_z \rangle_W = 0$$

$$\sum_{m_W} \langle m_W | \uparrow_z \rangle^*_W \langle m_W | \downarrow_z \rangle_W = w \langle \uparrow_z | \downarrow_z \rangle_W = 0$$

Therefore,

$$P(m_D) = \frac{1}{2} |\langle m_D | \uparrow_z \rangle_D|^2 + \frac{1}{2} |\langle m_D | \downarrow_z \rangle_D|^2$$

This probability distribution is a *statistical mixture* of probabilities arising from two different states $|\uparrow_z \rangle_D$ and $|\downarrow_z \rangle_D$.

This implies that the marginal state is a statistical mixture of pure states given by

$$\hat{\rho}_D = \frac{1}{2} (|\uparrow_z \rangle_D \langle \uparrow_z | + |\downarrow_z \rangle_D \langle \downarrow_z |)$$

(c) Suppose now the which-way detector does not function perfectly and does not completely flip the spin, but rotates it by an angle $\theta$ about $x$ so that

$$|\uparrow_\theta \rangle_W = \cos (\theta/2) |\uparrow_z \rangle_W + \sin (\theta/2) |\downarrow_z \rangle_W$$

Show that in this case the marginal state is

$$\hat{\rho}_D = \frac{1}{2} |\uparrow_\theta \rangle_D \langle \uparrow_\theta | + \frac{1}{2} |\downarrow_\theta \rangle_D \langle \downarrow_\theta |$$

$$+ \cos (\theta/2) |\uparrow_z \rangle_D \langle \downarrow_z | + \sin (\theta/2) |\downarrow_z \rangle_D \langle \uparrow_z |$$

Comment on the limits $\theta \to 0$ and $\theta \to \pi$.

We now consider a less perfect "which-way" detector which functions as

$$|\uparrow_z \rangle_D |\uparrow_z \rangle_W \rightarrow |\uparrow_z \rangle_D |\uparrow_\theta \rangle_W$$

$$|\downarrow_z \rangle_D |\uparrow_z \rangle_W \rightarrow |\downarrow_z \rangle_D |\downarrow_\theta \rangle_W$$
where
\[ |↑θ⟩_W = \cos(θ/2) |↑z⟩_W + \sin(θ/2) |↓z⟩_W \]

Note that
\[ \theta = 0 \Rightarrow \text{No interaction} \]
\[ \theta = π \Rightarrow \text{Full spin flip} \]

Again we have the composite state evolving as
\[ |↑x⟩_D |↑z⟩_W \Rightarrow \frac{1}{\sqrt{2}} |↑z⟩_D |↑z⟩_W + \frac{1}{\sqrt{2}} |↓z⟩_D |↑θ⟩_W = |Ψ_{DW}⟩ \]

The marginal probability distribution for D is
\[
P(m_D) = \sum_{m_W} |⟨m_D, m_W | Ψ_{DW}⟩|^2 = \frac{1}{2} \sum_{m_W} |⟨m_D | ↑z⟩_D⟩⟨m_W | ↑z⟩_W + ⟨m_D | ↓z⟩_D⟩⟨m_W | ↑θ⟩_W|^2
\]
\[= \frac{1}{2} |⟨m_D | ↑z⟩_D⟩|^2 \sum_{m_W} |⟨m_W | ↑z⟩_W|^2 + \frac{1}{2} |⟨m_D | ↓z⟩_D⟩|^2 \sum_{m_W} |⟨m_W | ↑θ⟩_W|^2
\]
\[+ \frac{1}{2} ⟨m_D | ↓z⟩_D^* ⟨m_D | ↑z⟩_D⟩ \sum_{m_W} ⟨m_W | ↑z⟩_W⟩⟨m_W | ↑z⟩_W
\]
\[+ \frac{1}{2} ⟨m_D | ↑z⟩_D^* ⟨m_D | ↓z⟩_D⟩ \sum_{m_W} ⟨m_W | ↑z⟩_W⟩⟨m_W | ↑θ⟩_W
\]

Now
\[\sum_{m_W} |⟨m_W | ↑z⟩_W|^2 = \sum_{m_W} |⟨m_W | ↑θ⟩_W|^2 = 1\]
\[\sum_{m_W} ⟨m_W | ↑z⟩_W⟩⟨m_W | ↑z⟩_W = w ⟨↑z | ↑z⟩_W = \cos θ\]
\[\sum_{m_W} ⟨m_W | ↑z⟩_W⟩⟨m_W | ↑θ⟩_W = w ⟨↑z | ↑θ⟩_W = \cos θ\]

so that
\[P(m_D) = \frac{1}{2} |⟨m_D | ↑z⟩_D⟩|^2 + \frac{1}{2} |⟨m_D | ↓z⟩_D⟩|^2
\]
\[+ \frac{1}{2} \cos θ \frac{1}{2} ⟨m_D | ↓z⟩_D^* ⟨m_D | ↑z⟩_D⟩ + \frac{1}{2} \cos θ \frac{1}{2} ⟨m_D | ↑z⟩_D^* ⟨m_D | ↓z⟩_D⟩
\]

This probability distribution arises from a density operator
\[\hat{ρ}_{m_D} = ⟨m_D | \hat{ρ}_D | m_D⟩\]

where
\[\hat{ρ}_D = \frac{1}{2} (|↑z⟩_D ⟨↑z| + |↓z⟩_D ⟨↓z|) + \frac{1}{2} \cos θ \frac{1}{2} (|↑z⟩_D ⟨↑z| + |↓z⟩_D ⟨↓z|)
\]
or in matrix form the density matrix is
\[\hat{ρ}_D = \frac{1}{2} \left( \begin{array}{cc} \cos \frac{θ}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{array} \right)\]
in the $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ basis.

Note that

$\theta \to \pi$: off-diagonal elements vanish and we get a completely mixed state.

$\theta \to 0$: off-diagonal elements are maximum and we get a pure state.

Upshot:

Feynman stated the rule:

"If two processes are in principle distinguishable (i.e., we can perform an experiment on some subsystem to see which process took place), then we add probabilities for the processes.

If two processes are indistinguishable (i.e., there exists no information to measure), then we add probability amplitudes."

We see how this works with the "which-way" detector. The paths are made distinguishable because $|\uparrow_z\rangle_W$ and $|\downarrow_z\rangle_W$ are orthogonal states. Thus, we could, in principle, measure electron $W$ to determine which path electron $D$ had taken.

The state $|\uparrow_z\rangle_W$ and $|\uparrow_\theta\rangle_W$ are not orthogonal states for $0 \leq \theta < \pi$, and thus, interference is only partially removed until $\theta \to \pi$.

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

$$\rho = \frac{1}{2} (|LL\rangle \langle LL| + |RR\rangle \langle RR|)$$

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 polar- 
ization. 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

$$\rho = \frac{1}{2} (|LL\rangle + |RR\rangle) (\langle LL| + \langle RR|)$$

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.

Yes, Oivil was just lucky. He will get it right every time in either case. Let us first define a basis so that we can see how it all works with explicit matrices. We have

\[
|LL\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix},
\ |LR\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix},
\ |RL\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix},
\ |RR\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\]

In this basis the density matrix for the first apparatus is:

$$\rho = \frac{1}{2} (|LL\rangle \langle LL| + |RR\rangle \langle RR|) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Since \( Tr(\rho^2) = 1/2 \), we know that this is a mixed state.

Now, Oivil observes that his photon is left-handed. His left-hand projection operator is

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

i.e.,

$$P_L |LL\rangle = |LL\rangle, \quad P_L |LR\rangle = |LR\rangle, \quad P_L |RL\rangle = 0, \quad P_L |RR\rangle = 0$$
so once he has made his measurement, the state has "collapsed" to

$$\rho_{after} = P_L \rho = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

This corresponds to a pure $|LL\rangle$ state. Hence, Livio will observe left-handed polarization.

For the second apparatus, the density matrix is

$$\rho = \frac{1}{2} (|LL\rangle + |RR\rangle)(\langle LL| + \langle RR|) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

Since $Tr(\rho^2) = 1$, we know that this is a pure state. Applying the left-handed projection for Oivil’s photon, we again obtain:

$$\rho_{after} = P_L \rho = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Again, Livio will observe left-handed polarization.

(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.

Livio’s left-handed projection operator is

$$P_L(\text{Livio}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The probability that Livio will observe a left-handed photon for the first
The same result is obtained for the second apparatus.

Here is my take on the philosophical issue (beware!):

If causality means propagation of information faster than the speed of light, then the answer is "no", causality is not violated. Oivil has not propagated any information to Livio at superluminal speeds. Livio made his own observation on the state of the system. Notice that the statistics of Livio’s observations are unaltered; independent of what Oivil does, he will still see left-handed photons 50% of the time. If this were not the case, then there would be a problem, since Oivil could exploit this to propagate a message to Livio long after the photons are emitted.

However, people widely interpret (and write flashy headlines) this sort of effect as a kind of "action at a distance". By measuring the state of his photon, Oivil instantly "kicks" Livio’s far off photon into a particular state (without being usable for the propagation of information, since Oivil can’t tell Livio about anything faster than the speed of light). Note that this philosophical dilemma is not silly: the wave function for Livio’s photon has both left- and right-handed components; how could a measurement of Oivil’s photon "pick" which component Livio will see?

Because of this, quantum mechanics is often labelled "non-local".

On the other hand, this philosophical perspective may be avoided (ignored) - it may be suggested that it doesn’t make sense to talk this way about the "wave function" of Livio’s photon, since the specification of the wave function also involves Oivil’s photon. Oivil is merely making a measurement of the state of the two-photon system, by observing the polarization of one of the photons, and knowing the coherence of the system. He doesn’t need to make two measurements to know both polarizations, they are completely correlated. Nothing is causing anything else to happen at faster than light speed. We might take the (deterministic?) point of view that it was already determined at production which polarization
Livio would see for a particular photon - we just don't know what it will be unless Oivil makes his measurement. There appears to be no way of falsifying this point of view, as stated. However, taking this point of view leads to the further philosophical question of how the pre-determined information is encoded - is the photon propagating towards Livio somehow carrying the information that it is going to be measured as left-handed? This conclusion seems hard to avoid. It leads to the notion of "hidden variables", and there are theories of this sort, which are testable.

We know that our quantum mechanical foundations are compatible with special relativity, hence with the notion of causality that implies.

As Feynman remarked in a seminar concerning EPR, the substantive question to be asking is,

"Do the predictions of quantum mechanics agree with experiment?"

So far the answer is a resounding "yes". Indeed, we often rely heavily on this quantum coherence in carrying out other research activities.

15.6.8 Measurements on Qubits

You are given one of two quantum states of a single qubit (physical system representing a 2-valued state): either $|\phi\rangle = |0\rangle$ or $|\phi\rangle = \cos \theta |0\rangle + \sin \theta |1\rangle$. You want to make a single measurement that best distinguishes between these two states, i.e., you want to find the best basis for making a measurement to distinguish the two states. So let us measure the qubit in the basis \{ $|\nu\rangle = \alpha |0\rangle + \beta |1\rangle$, $|\nu^\perp\rangle$ \}, where $\alpha$, $\beta$ are to be determined for optimal success. For outcome $|\nu\rangle$ we guess that the qubit was in state $|0\rangle$; for outcome $|\nu^\perp\rangle$ we guess that the qubit was in state $|\phi\rangle$. Determine the optimal measurement basis given this procedure. You can take $\alpha$ and $\beta$ to be real numbers, in which case the normalization $|\alpha|^2 + |\beta|^2 = 1$ implies that you can write $\alpha$ and $\beta$ 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

$$Pr[\text{qubit was } |0\rangle]Pr[|\nu\rangle |\text{qubit was } |0\rangle] + Pr[\text{qubit was } |\psi\rangle]Pr[|\nu^\perp\rangle |\text{qubit was } |\psi\rangle]$$

where, e.g.

$$Pr[|\nu\rangle |\text{qubit was } |0\rangle] = |\langle \nu | 0 \rangle|^2$$

If the state you are presented with is either $|\phi\rangle$ or $|\psi\rangle$ with 50% probability each, what is the probability that your measurement correctly identifies the state?

We measure the qubit in basis $|\nu\rangle = \alpha |0\rangle + \beta |1\rangle$, $|\nu^\perp\rangle$. For outcome $|\nu\rangle$ we guess that the qubit was in state $|0\rangle$; for outcome $|\nu^\perp\rangle$ we guess that the qubit was in the state $|\psi\rangle$. 688
The optimal measurement basis is $|\nu\rangle = \cos \gamma |0\rangle + \sin \gamma |1\rangle$, where $\gamma = (\theta - \pi/2)/2$. Graphically, this means that the angle bisector between $|\nu\rangle$ and $|\nu^\perp\rangle$ is the same as between $|0\rangle$ and $|\psi\rangle$.

Let us prove that this choice of measurement basis $|\nu\rangle, |\nu^\perp\rangle$ indeed maximizes the probability that our guess is correct: now

$$
Pr[qubit was |0\rangle]Pr[|\nu\rangle |qubit was |0\rangle] + Pr[qubit was |\psi\rangle]Pr[|\nu^\perp\rangle |qubit was |\psi\rangle] = \frac{1}{2} (|\langle \nu | 0 \rangle|^2 + |\langle \nu^\perp | \psi \rangle|^2)
$$

Let $|\nu\rangle = \alpha |0\rangle + \beta |1\rangle$. We want to choose $\alpha, \beta$ to maximize

$$
|\langle \nu | 0 \rangle|^2 - |\langle \nu | \psi \rangle|^2 = |\alpha|^2 - |\alpha \cos \theta + \beta \sin \theta|^2
$$

Using $1 - \cos^2 \theta = \sin^2 \theta$ and assuming without loss of generality $\sin \theta \geq 0$, this is equivalent to maximizing

$$
\sin \theta (|\alpha|^2 - |\beta|^2) - \cos \theta (\alpha^* \beta + \alpha \beta^*)
$$

We may assume $\alpha, \beta \in \mathbb{R}$, since for fixed magnitudes $|\alpha|, |\beta|$, we want to choose arguments such as to either maximize (if $\cos \theta < 0$) or minimize (if $\cos \theta > 0$) the real part of $\alpha^* \beta$. Therefore, let $\alpha = \cos \gamma, \beta = \sin \gamma$ for some angle $\gamma$. Then we wish to maximize

$$
\sin \theta \cos 2\gamma - \cos \theta \sin 2\gamma = \sin (\theta - 2\gamma)
$$

Therefore, let

$$
\gamma = \frac{1}{2} \left( \theta - \frac{\pi}{2} \right)
$$

Geometrically, the vector $|\nu\rangle + |\nu^\perp\rangle$ is a multiple of $|0\rangle + |\psi\rangle$.

The success probability with this choice of $\gamma$ is

$$
\cos^2 \left( \frac{\pi}{4} - \frac{\theta}{2} \right) = \frac{1}{2} (1 + \sin \theta)
$$

Without the assumption $\sin \theta > 0$, the success probability is

$$
\frac{1}{2} (1 + |\sin \theta|)
$$

Any two quantum states, in an arbitrary dimension, lie in a plane. By rotational symmetry the above argument applies: the optimal measurement gives a success probability of

$$
\frac{1}{2} (1 + \sqrt{1 - |\langle \phi | \psi \rangle|^2})
$$
Note that this probability is 1 if $|\phi\rangle$ and $|\psi\rangle$ are orthogonal, hence perfectly distinguishable. This probability is $1/2$ if $|\langle \phi | \psi \rangle| = 1$. In this case there is no optimal basis, you can do no better than just randomly guessing.

Note that allowing multiple measurements does not increase the optimum success probability - only the first measurement gives information about the original state. Also, a unitary transformation, followed by a measurement, is the same as a measurement in a rotated basis - so allowing unitary transformations does not increase the optimum success probability either.

15.6.9 To be entangled....

Let $\mathcal{H}_A = \text{span}\{|0_A\rangle, |1_A\rangle\}$ and $\mathcal{H}_B = \text{span}\{|0_B\rangle, |1_B\rangle\}$ 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

$$U_{AB} = |0_A\rangle \langle 0_A| \otimes |0_B\rangle \langle 0_B| - |1_A\rangle \langle 1_A| \otimes |1_B\rangle \langle 1_B|$$

Since it is factorizable, we can write:

$$|\Psi_{AB}\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle = (a_0 |0_A\rangle + a_1 |1_A\rangle) \otimes (b_0 |0_B\rangle + b_1 |1_B\rangle)$$

where the coefficients $(a_0, a_1, b_0, b_1)$ are complex numbers.

Now

$$U_{AB} |\Psi_{AB}\rangle = (a_0 |0_A\rangle \otimes (b_0 |0_B\rangle) - (a_1 |1_A\rangle \otimes (b_1 |1_B\rangle))$$

and therefore

$$U_{AB} |\Psi_{AB}\rangle = a_0 b_0 |0_A\rangle \otimes |0_B\rangle - a_1 b_1 |1_A\rangle \otimes |1_B\rangle$$

This new state is entangled if and only if both $a_0 b_0$ and $a_1 b_1$ are non-vanishing (i.e., if one of these is zero, then the state is trivially factorizable, and if the state is factorizable, then one of these must be zero).

This is the same condition that all $a_0, a_1, b_0, b_1$ are nonzero, or that $\langle 0_A 0_B | \Psi_{AB}\rangle$ and $\langle 1_A 1_B | \Psi_{AB}\rangle$ are both nonzero.

To see explicitly that this new state is factorizable if and only if at least one of $a_0 b_0$ or $a_1 b_1$ is zero, consider it purity: we have

$$\rho = U_{AB} |\Psi_{AB}\rangle \langle \Psi_{AB}| U_{AB}$$

$$\tilde{\rho}_A = TR_B[\rho] = |a_0 b_0|^2 |0_A\rangle \langle 0_A| + |a_1 b_1|^2 |1_A\rangle \langle 1_A|$$

$$TR[\rho] = TR_B[\tilde{\rho}_A] = |a_0 b_0|^2 + |a_1 b_1|^2 = 1$$

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\[ \rho_A^2 = |a_0 b_0|^2 |0_A\rangle \langle 0_A| + |a_1 b_1|^2 |1_A\rangle \langle 1_A| \]
\[ \zeta = Tr_A[\rho_A^2] = |a_0 b_0|^4 + |a_1 b_1|^4 \]

Thus, if \( \zeta = 1 \) (i.e., the state is factorizable), then
\[ |a_0 b_0|^2 + |a_1 b_1|^2 = |a_0 b_0|^4 + |a_1 b_1|^4 \]

The only solutions of this equation subject to the constraints \( 0 \leq \{|a_0 b_0|, |a_1 b_1|\} \leq 1 \) (this follows from assuming that \( |\Psi_{AB}\rangle \) is normalized, which is always assumed when considering \( \zeta \)) are:
- \( |a_0 b_0| = 1 \), \( |a_1 b_1| = 1 \)
- \( |a_0 b_0| = 0 \), \( |a_1 b_1| = 1 \)
- \( |a_0 b_0| = 0 \), \( |a_1 b_1| = 0 \)

### 15.6.10 Alice, Bob and Charlie

Let Alice, Bob and Charlie be in possession of quantum systems whose states live in \( H_A = \text{span}\{|0_A\rangle, |1_A\rangle\} \), \( H_B = \text{span}\{|0_B\rangle, |1_B\rangle\} \) and \( H_C = \text{span}\{|0_C\rangle, |1_C\rangle\} \), respectively. Suppose that a joint state of these systems has been prepared as the (three-way) entangled state
\[ |\Psi_{ABC}\rangle = \frac{1}{\sqrt{2}} (|0_A0_B0_C\rangle + |1_A1_B1_C\rangle) \]

(a) What is the reduced density operator on \( H_A \otimes H_B \) if we take a partial trace over \( H_C \)?
\[ \rho = |\Psi_{ABC}\rangle \langle \Psi_{ABC}| \]
\[ = \frac{1}{2} (|0_A0_B0_C\rangle \langle 0_A0_B0_C| + |0_A0_B0_C\rangle \langle 1_A1_B1_C| + |1_A1_B1_C\rangle \langle 0_A0_B0_C| + |1_A1_B1_C\rangle \langle 1_A1_B1_C|) \]

and
\[ \hat{\rho}_{AB} = Tr_C[\rho] = \sum_{k=0,1} \langle k_C| \rho |k_C\rangle = \frac{1}{2} (|0_A0_B\rangle \langle 0_A0_B| + |1_A1_B\rangle \langle 1_A1_B|) \]

(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)

Let
\[ P_0 = I_A \otimes I_B \otimes |0_C\rangle \langle 0_C| \]
\[ P_1 = I_A \otimes I_B \otimes |1_C\rangle \langle 1_C| \]
Then
\[ Pr(0) = Tr[|P_0\rangle\langle P_0|] = Tr \left[ \frac{1}{2} (|0_A0B0_C\rangle \langle 0_A0B0_C| + |1_A1B1_C\rangle \langle 1_A1B1_C|) \right] = \frac{1}{2} \]
\[ Pr(1) = Tr[|P_1\rangle\langle P_1|] = Tr \left[ \frac{1}{2} (|1_A1B1_C\rangle \langle 0_A0B0_C| + |1_A1B1_C\rangle \langle 1_A1B1_C|) \right] = \frac{1}{2} \]

With post-measurement states:
\[ |\Psi_0\rangle = \frac{P_0|\Psi_{ABC}\rangle}{\langle \Psi_{ABC}|P_0|\Psi_{ABC}\rangle} = \frac{P_0|\Psi_{ABC}\rangle}{\sqrt{Tr[|P_0\rangle\langle P_0|]}} = \frac{|0_A0B0_C\rangle}{\sqrt{2}} \]
\[ |\Psi_1\rangle = \frac{P_1|\Psi_{ABC}\rangle}{\langle \Psi_{ABC}|P_1|\Psi_{ABC}\rangle} = \frac{P_1|\Psi_{ABC}\rangle}{\sqrt{Tr[|P_1\rangle\langle P_1|]}} = \frac{|1_A1B1_C\rangle}{\sqrt{2}} \]

This is consistent with the result from (a) since
\[ \rho^{01} = Pr(0) |\Psi_0\rangle \langle \Psi_0| + Pr(1) |\Psi_1\rangle \langle \Psi_1| \]
\[ = \frac{1}{2} (|0_A0B0_C\rangle \langle 0_A0B0_C| + |1_A1B1_C\rangle \langle 1_A1B1_C|) \]
\[ \hat{\rho}^{(0)}_{AB} = Tr_C[|p_{pm}\rangle\langle p_{pm}|] = \frac{1}{2} (|0_A0B\rangle \langle 0_A0B| + |1_A1B\rangle \langle 1_A1B|) = \hat{\rho}^{AB} \]

(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
\[ |x_C\rangle = \frac{1}{\sqrt{2}} (|0_C\rangle + |1_C\rangle) \]
\[ |y_C\rangle = \frac{1}{\sqrt{2}} (|0_C\rangle - |1_C\rangle) \]

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).

Let
\[ P_x = I_A \otimes I_B \otimes |x_C\rangle \langle x_C| \]
\[ P_y = I_A \otimes I_B \otimes |y_C\rangle \langle y_C| \]

Then
\[ Pr(x) = Tr[|P_x\rangle\langle P_x|] = \frac{1}{2} \]
\[ Pr(y) = Tr[|P_y\rangle\langle P_y|] = \frac{1}{2} \]

With post-measurement states:
\[ |\Psi_x\rangle = \frac{P_x|\Psi_{ABC}\rangle}{\langle \Psi_{ABC}|P_x|\Psi_{ABC}\rangle} = \frac{P_x|\Psi_{ABC}\rangle}{\sqrt{Tr[|P_x\rangle\langle P_x|]}} \]
\[ = \frac{1}{2} (|0_A0B0_C\rangle + |0_A0B1_C\rangle + |1_A1B0_C\rangle + |1_A1B1_C\rangle) \]
\[ = \frac{1}{\sqrt{2}} (|0_A0B\rangle + |1_A1B\rangle) \otimes |x_C\rangle \]
\[ |\Psi_y\rangle = \frac{P_y|\Psi_{ABC}\rangle}{\langle \Psi_{ABC}|P_y|\Psi_{ABC}\rangle} = \frac{P_y|\Psi_{ABC}\rangle}{\sqrt{Tr[|P_y\rangle\langle P_y|]}} \]
\[ = \frac{1}{2} (|0_A0B0_C\rangle - |0_A0B1_C\rangle - |1_A1B0_C\rangle + |1_A1B1_C\rangle) \]
\[ = \frac{1}{\sqrt{2}} (|0_A0B\rangle - |1_A1B\rangle) \otimes |y_C\rangle \]
This is consistent with the result from (a) since

$$\rho^{xy} = Pr(x) |\Psi_x\rangle \langle \Psi_x| + Pr(y) |\Psi_y\rangle \langle \Psi_y|$$

$$= \frac{1}{4} (|0_A0_B\rangle + |1_A1_B\rangle)(|0_A0_B\rangle + |1_A1_B\rangle) \otimes |x_C\rangle \langle x_C|$$

$$+ \frac{1}{4} (|0_A0_B\rangle - |1_A1_B\rangle)(|0_A0_B\rangle - |1_A1_B\rangle) \otimes |y_C\rangle \langle y_C|)$$

$$\tilde{\rho}_{AB}^{xy} = Tr_C [\rho^{pm}] = |x_C\rangle \langle x_C| + |y_C\rangle \langle y_C|$$

$$= \frac{1}{4} (|0_A0_B\rangle + |1_A1_B\rangle)(|0_A0_B\rangle + |1_A1_B\rangle) + \frac{1}{4} (|0_A0_B\rangle - |1_A1_B\rangle)(|0_A0_B\rangle - |1_A1_B\rangle)$$

$$= \frac{1}{2} (|0_A0_B\rangle \langle 0_A0_B| + |1_A1_B\rangle \langle 1_A1_B|) = \tilde{\rho}_{AB}$$

(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 $H_A \otimes H_B$. 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?

Assuming equal probabilities for Charlie’s two measurement bases, the ensemble on $H_A \otimes H_B$ will be:

- $|0_{AB}\rangle = |0_A0_B\rangle$ with $Pr(0_{AB}) = \frac{1}{4}$
- $|1_{AB}\rangle = |1_A1_B\rangle$ with $Pr(1_{AB}) = \frac{1}{4}$
- $|x_{AB}\rangle = \frac{1}{\sqrt{2}} (|0_A0_B\rangle + |1_A1_B\rangle)$ with $Pr(x_{AB}) = \frac{1}{4}$
- $|y_{AB}\rangle = \frac{1}{\sqrt{2}} (|0_A0_B\rangle - |1_A1_B\rangle)$ with $Pr(y_{AB}) = \frac{1}{4}$

$$\rho^{pm}_{AB} = \frac{1}{4} (|0_{AB}\rangle \langle 0_{AB}| + |1_{AB}\rangle \langle 1_{AB}| + |x_{AB}\rangle \langle x_{AB}| + |y_{AB}\rangle \langle y_{AB}|)$$

$$= \frac{1}{2} (|0_A0_B\rangle \langle 0_A0_B| + |1_A1_B\rangle \langle 1_A1_B|) = \tilde{\rho}_{AB}$$

We can also use the results from (b) and (c) to write the post-measurement density operator on $H_A \otimes H_B \otimes H_C$ and its reduced density operator on $H_A \otimes H_B$:

$$\rho^{pm}_{AB} = Pr(01 - basis) \rho^{01} + Pr(xy - basis) \rho^{xy} = \frac{1}{2} \rho^{01} + \frac{1}{2} \rho^{xy}$$

$$\frac{1}{2} (|0_C\rangle \rho^{01} |0_C\rangle + |1_C\rangle \rho^{01} |1_C\rangle + |x_C\rangle \rho^{01} |x_C\rangle + |y_C\rangle \rho^{01} |y_C\rangle)$$

$$= \frac{1}{2} (\tilde{\rho}_{AB} + \tilde{\rho}_{AB}) = \tilde{\rho}_{AB}$$

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So these are all consistent with the result from (a).

If Charlie informs Alice and Bob of which measurement he performed and the outcome, then the post-measurement state on $H_A \otimes H_B$ is completely determined, so Alice and Bob should change their ensemble description to be probability of 1 in the unique state. Specifically:

If Charlie measured $|0_C\rangle$ in the 01− basis, then $|0_{AB}\rangle$ with $Pr(0_{AB}) = 1$

If Charlie measured $|1_C\rangle$ in the 01− basis, then $|1_{AB}\rangle$ with $Pr(1_{AB}) = 1$

If Charlie measured $|x_C\rangle$ in the $xy$− basis, then $|x_{AB}\rangle$ with $Pr(x_{AB}) = 1$

If Charlie measured $|y_C\rangle$ in the $xy$− basis, then $|y_{AB}\rangle$ with $Pr(y_{AB}) = 1$
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).

![EPR Stern-Gerlach Setup](image)

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

\[
\sigma^{(1)} = \frac{2}{\hbar} \hat{n}_1 \cdot \vec{S}_1, \quad \sigma^{(2)} = \frac{2}{\hbar} \hat{n}_2 \cdot \vec{S}_2
\]

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?

The eigenstates and the corresponding quantum numbers relating to \(\sigma^{(1)}\)
and $\sigma^{(2)}$ are

\[ \begin{align*}
|S_{n_1}+\rangle^{(1)}|S_{n_2}+\rangle^{(2)} &+ 1, +1 \\
|S_{n_1}-\rangle^{(1)}|S_{n_2}+\rangle^{(2)} &- 1, +1 \\
|S_{n_1}+\rangle^{(1)}|S_{n_2}-\rangle^{(2)} &+ 1, -1 \\
|S_{n_1}-\rangle^{(1)}|S_{n_2}-\rangle^{(2)} &- 1, -1
\end{align*} \]

where the spin eigenstates for a general direction can be expressed in terms of the standard eigenstates with respect to $z$ as

\[ \begin{align*}
|S_n+\rangle &= \cos \frac{\phi}{2} |S_z+\rangle + i \sin \frac{\phi}{2} |S_z-\rangle \\
|S_n-\rangle &= i \sin \frac{\phi}{2} |S_z+\rangle + \cos \frac{\phi}{2} |S_z-\rangle
\end{align*} \]

The inverse relations are:

\[ \begin{align*}
|S_z+\rangle &= \cos \frac{\phi}{2} |S_n+\rangle - i \sin \frac{\phi}{2} |S_n-\rangle \\
|S_z-\rangle &= -i \sin \frac{\phi}{2} |S_n+\rangle + \cos \frac{\phi}{2} |S_n-\rangle
\end{align*} \]

The angle $\phi$ equals $\cos^{-1}(\hat{n} \cdot \hat{z})$.

(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

\[ |0,0\rangle = \frac{1}{\sqrt{2}} (|S_z+\rangle^{(1)}|S_z-\rangle^{(2)} - |S_z-\rangle^{(1)}|S_z+\rangle^{(2)}) \]

What is the expectation value of $\sigma^{(12)}$?

The eigenvectors of $\sigma^{(12)}$ are the same as those of $\sigma^{(1)}$ and $\sigma^{(2)}$. The corresponding quantum numbers are the products of the pairs of quantum numbers in (a):

\[ \begin{align*}
|S_{n_1}+\rangle^{(1)}|S_{n_2}+\rangle^{(2)} &+ 1 \\
|S_{n_1}-\rangle^{(1)}|S_{n_2}+\rangle^{(2)} &- 1 \\
|S_{n_1}+\rangle^{(1)}|S_{n_2}-\rangle^{(2)} &- 1 \\
|S_{n_1}-\rangle^{(1)}|S_{n_2}-\rangle^{(2)} &+ 1
\end{align*} \]

The state of the pair is given as the singlet

\[ |00\rangle = \frac{1}{\sqrt{2}} (|S_z+\rangle^{(1)}|S_z-\rangle^{(2)} - |S_z-\rangle^{(1)}|S_z+\rangle^{(2)}) \]

Therefore, using,

\[ \begin{align*}
\langle S_z\pm|\sigma^{(i)}|S_z\pm \rangle &= \pm \cos \phi_i \\
\langle S_z\pm|\sigma^{(i)}|S_z\mp \rangle &= \mp i \sin \phi_i
\end{align*} \]

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the expectation value of $\sigma^{(12)}$ will be

\[
\langle 00|\sigma^{(12)}|00\rangle = \langle 00|\sigma^{(1)}|00\rangle \langle 00|\sigma^{(2)}|00\rangle \\
= \frac{1}{2} \langle S_z^+|\sigma^{(1)}|S_z^+\rangle \langle S_z^-|\sigma^{(2)}|S_z^-\rangle \\
- \frac{1}{2} \langle S_z^+|\sigma^{(1)}|S_z^-\rangle \langle S_z^-|\sigma^{(2)}|S_z^+\rangle \\
- \frac{1}{2} \langle S_z^-|\sigma^{(1)}|S_z^+\rangle \langle S_z^+|\sigma^{(2)}|S_z^-\rangle \\
+ \frac{1}{2} \langle S_z^-|\sigma^{(1)}|S_z^-\rangle \langle S_z^-|\sigma^{(2)}|S_z^+\rangle \\
= -\cos \phi_1 \cos \phi_2 + \sin \phi_1 \sin \phi_2 = -\cos (\phi_1 - \phi_2) = -\hat{n}_1 \cdot \hat{n}_2
\]

\[(c) \text{ Make the assumption that the spin of a particle has a meaningful value even when it is not being measured. Assume also that the only possible results of the measurement of a spin component are } \pm \frac{\hbar}{2}. \text{ Then show that the probability of finding the spins pointing in two given directions will be proportional to the overlap of the hemispheres that these two directions define. Quantify this criterion and calculate the expectation value of } \sigma^{(12)}.\]

The expectation value of $\sigma^{(12)}$ in this scheme would be

\[
\langle \sigma^{(12)} \rangle = P_{++} + P_{--} - P_{+-} - P_{-+}
\]

where $P_{++}$ is the probability that both particles have their spin 'up' with respect to the field direction in the corresponding Stern-Gerlach apparatus. Similarly, for the rest of the probabilities. Each particle, by assumption has a well-defined spin independently of observation. If a spin component of a particle has been measured as $+\frac{\hbar}{2}$ then we can conclude that its spin will lie somewhere in the hemisphere defined by this 'up' direction. Obviously, the spin of the other particle will lie in the 'down' hemisphere. The spin directions are shown below.

Consider the spin components of the two particles along directions that make an angle $\phi$. The probability of finding the spin components of both
particles to be $+\hbar/2$ will be proportional to the overlap of their corresponding 'up' hemispheres,

$$P_{++} = \frac{\phi}{\pi} = P_{--}$$

The proportionality coefficient is determined by the fact that the probability must be equal to 1 when $\phi = \pi$.

The probability of finding the two spin components pointing in opposite directions can be written as

$$P_{+-} = a\phi + b$$

This probability would be 1 if the two hemispheres coincided ($\phi = 0$); thus, $b = 1$. It vanishes if $\phi = \pi$, however. Thus, $a = -1/\pi$. Therefore

$$P_{+-} = P_{-+} = 1 - \frac{\phi}{\pi}$$

Finally we get

$$\langle \sigma^{(12)} \rangle = 2\frac{\phi}{\pi} - 2 \left( 1 - \frac{\phi}{\pi} \right) = \frac{4}{\pi} \left( \phi - \frac{\pi}{2} \right)$$

(d) Assume the spin variables depend on a hidden variable $\lambda$. The expectation value of the spin observable $\sigma^{(12)}$ is determined in terms of the normalized distribution function $f(\lambda)$:

$$\left\langle \sigma^{(12)} \right\rangle = \frac{4}{\hbar^2} \int d\lambda f(\lambda) S_z^{(1)}(\lambda) S_z^{(2)}(\lambda)$$

Prove Bell’s inequality

$$\left| \left\langle \sigma^{(12)}(\varphi) \right\rangle - \left\langle \sigma^{(12)}(\varphi') \right\rangle \right| \leq 1 + \left| \left\langle \sigma^{(12)}(\varphi - \varphi') \right\rangle \right|$$

We have

$$\left\langle \sigma^{(12)}(\varphi) \right\rangle - \left\langle \sigma^{(12)}(\varphi') \right\rangle = \frac{4}{\hbar^2} \int d\lambda f(\lambda) S_z^{(1)}(\lambda)(S_z^{(2)}(\lambda) - S_z^{(2)}(\lambda))$$

$$= -4 \frac{\hbar^2}{\hbar^2} \int d\lambda f(\lambda) S_z^{(1)}(\lambda) S_z^{(1)}(\lambda)$$

$$+ 16 \frac{\hbar^2}{\hbar^2} \int d\lambda f(\lambda) S_z^{(1)}(\lambda) S_z^{(1)}(\lambda) S_z^{(2)}(\lambda) S_z^{(2)}(\lambda)$$

$$= -4 \frac{\hbar^2}{\hbar^2} \int d\lambda f(\lambda) S_z^{(1)}(\lambda) S_z^{(1)}(\lambda) \left( 1 - 4 \frac{\hbar^2}{\hbar^2} S_z^{(2)}(\lambda) S_z^{(2)}(\lambda) \right)$$

where we have used

$$S_z^{(2)}(\lambda) = -S_z^{(1)}(\lambda) \quad , \quad [S_z^{(1)}(\lambda)]^2 = \frac{\hbar^2}{4}$$
The last equality gives the inequality
\[
\left| \left\langle \sigma^{(12)}(\varphi) \right| - \left\langle \sigma^{(12)}(\varphi') \right| \right| \leq \frac{4}{\hbar^2} \int d\lambda f(\lambda) \left| S^{(1)}(\lambda)S^{(1)}_{\varphi} \right| \left| \left( 1 - \frac{4}{\hbar^2} S^{(2)}(\lambda)S^{(2)}_{\varphi'} \right) \right|
\]
\[
= \int d\lambda f(\lambda) \left( 1 - \frac{4}{\hbar^2} S^{(2)}(\lambda)S^{(2)}_{\varphi'} \right)
\]

Note that the quantity in square brackets is positive. Thus, we finally have
\[
\left| \left\langle \sigma^{(12)}(\varphi) \right| - \left\langle \sigma^{(12)}(\varphi') \right| \right| \leq 1 + \left\langle \sigma^{(12)}(\varphi - \varphi') \right| \right|
\]

(e) Consider Bell’s inequality for \( \varphi' = 2\varphi \) and show that it is not true when applied in the context of quantum mechanics.

Although Bell’s inequality was derived in the framework of a so-called local hidden variable theory, let us apply it in quantum mechanics in the specific case \( \varphi' = 2\varphi \). Using the quantum mechanical result found in part (b) we get
\[
\left\langle \sigma^{(12)} \right| = -\cos \varphi
\]

Bell’s inequality then implies that
\[
|\cos \varphi - \cos 2\varphi| \leq 1 - \cos \varphi
\]

This, however, is not true in the region \( 0 < \varphi < \pi/2 \). Since experiment has confirmed the quantum mechanical predictions for all values of \( \varphi \) and \( \varphi' \), this immediately implies that the whole framework of local hidden variable theories is ruled out.

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 \( \lambda \) 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 \(|B| \leq 2\)

With the separability assumption, we have

\[
C(\hat{a}, \hat{b}) = \int d\lambda \rho(\lambda) C(\hat{a}, \lambda) C(\hat{b}, \lambda)
\]

It follows that the Bell coefficient can be written in the form

\[
B = C(\hat{a}, \hat{b}) + C(\hat{a}, \hat{b}') + C(\hat{a}', \hat{b}) - C(\hat{a}', \hat{b}')
\]

\[
= \int d\lambda \rho(\lambda) \left( C(\hat{a}, \lambda)(C(\hat{b}, \lambda) + C(\hat{b}', \lambda)) + C(\hat{a}', \lambda)(C(\hat{b}, \lambda) - C(\hat{b}', \lambda)) \right)
\]

Since \(|C(\hat{a}, \lambda)| \leq 1\), \(|C(\hat{a}', \lambda)| \leq 1\) and \( \rho(\lambda) \geq 0 \), we have

\[
|B| \leq \int d\lambda \rho(\lambda) \left( \left| C(\hat{b}, \lambda) + C(\hat{b}', \lambda) \right| + \left| C(\hat{b}, \lambda) - C(\hat{b}', \lambda) \right| \right)
\]

Now suppose that for a given \( \lambda \), \( C_M(\lambda) \) is the maximum and \( C_m(\lambda) \) is the minimum of \( C(\hat{b}, \lambda) \) and \( C(\hat{b}', \lambda) \), so that \( C_M(\lambda) \geq C_m(\lambda) \). Then

\[
|B| \leq \int d\lambda \rho(\lambda) \left( |C_M(\lambda) + C_m(\lambda)| + C_M(\lambda) - C_m(\lambda) \right)
\]
There are two cases to consider.

For the case $C_M(\lambda) \geq 0$, we have $|C_M(\lambda) + C_m(\lambda)| = C_M(\lambda) + C_m(\lambda)$ so that

$$|B| \leq \int d\lambda \rho(\lambda) (C_M(\lambda) + C_m(\lambda) + C_M(\lambda) - C_m(\lambda))$$

$$= 2 \int d\lambda \rho(\lambda) C_M(\lambda) \leq 2 \int d\lambda \rho(\lambda) |C_M(\lambda)| \leq 2 \int d\lambda \rho(\lambda) = 2$$

For the case $C_M(\lambda) < 0$, we have $|C_M(\lambda) + C_m(\lambda)| = -C_M(\lambda) - C_m(\lambda)$ so that

$$|B| \leq \int d\lambda \rho(\lambda) (-C_M(\lambda) - C_m(\lambda) + C_M(\lambda) - C_m(\lambda))$$

$$= 2 \int d\lambda \rho(\lambda) (-C_m(\lambda)) \leq 2 \int d\lambda \rho(\lambda) |C_m(\lambda)| \leq 2 \int d\lambda \rho(\lambda) = 2$$

Thus, in all cases $|B| \leq 2$.

(2) Show that quantum mechanics predicts that $C(\hat{a}, \hat{b}) = 2(\hat{a} \cdot \hat{b})^2 - 1$

A photon, traveling in the $y$ direction, might have right- or left-handed circular polarization. The corresponding quantum states are written $|R\rangle$ and $|L\rangle$ respectively. These circular polarization states can be expressed as coherent superpositions of linearly polarized states in the $z$ and $x$ directions:

$$|R\rangle = \frac{1}{\sqrt{2}} (|z\rangle + i |x\rangle)$$

$$|L\rangle = \frac{1}{\sqrt{2}} (|z\rangle - i |x\rangle)$$

Under a rotation of the coordinate axes by an angle $\theta$ about the $y$ direction, $|R\rangle \rightarrow e^{i\theta} |R\rangle$ and $|L\rangle \rightarrow e^{-i\theta} |L\rangle$ or equivalently

$$\begin{pmatrix}
|z\rangle \\
|x\rangle
\end{pmatrix} \rightarrow \begin{pmatrix}
|z'\rangle \\
|x'\rangle
\end{pmatrix} = \begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix} \begin{pmatrix}
|z\rangle \\
|x\rangle
\end{pmatrix}$$

If each photon is in a state of right-handed circular polarization, we write the corresponding state vector as $|R_1\rangle |R_2\rangle$.

However, since the photons are moving in opposite directions, one along the positive, and the other along the negative $y$ axis, it follows that the actual directions in which the electric fields rotate, in time, in the vicinity of the two photons, are opposed to one another. The same hold for the state $|L_1\rangle |L_2\rangle$, corresponding to each photon being in a state of left-handed circular polarization.

The linear combination of these two states,

$$|EPR\rangle = \frac{1}{\sqrt{2}} (|R_1\rangle |R_2\rangle + |L_1\rangle |L_2\rangle)$$
corresponds to the more general situation in which the photons are in oppositely oriented states of circular polarization, where the sense of this polarization is not specified. We can write this entangled or Einstein-Podolsky-Rosen state in the form

$$|EPR⟩ = \frac{1}{\sqrt{2}} (|z_1⟩ |z_2⟩ − |x_1⟩ |x_2⟩)$$

which is a superposition of states of linear polarization.

Suppose now that a measurement of linear polarization is made on photon 1 in the $z$ direction, and of photon 2 in the $z$ direction, that is, the $z$ direction after a rotation of the axes about the $y$ axis. The probability amplitude associated with this measurement on the EPR state is

$$⟨EPR| z'_1 z'_2⟩ = \frac{1}{\sqrt{2}} (⟨z_1| ⟨z_2| − ⟨x_1| ⟨x_2|) (⟨z_1| (\cos θ |z_2⟩ − \sin θ |x_2⟩)) = \frac{1}{\sqrt{2}} \cos θ$$

where we have used $⟨z_1| x_1⟩ = 0$. The probability that photon 1 is found to have linear polarization in the direction $z$, and photon 2 in the direction $z$ is

$$P_{++}(\hat{a}, \hat{b}) = |⟨EPR| z_1 z'_2⟩|^2 = \frac{1}{2} \cos^2 θ$$

where we have assumed that $\hat{a}$ is in the $z$ direction and $\hat{b}$ is in the $z'$ direction.

Suppose next that the linear polarization of the linear polarization of photon 1 were measured in the $x$ direction, and that of photon 2 again in the $z$ direction. The probability amplitude is

$$⟨EPR| x_1 z'_2⟩ = \frac{1}{\sqrt{2}} ((⟨z_1| ⟨z_2| − ⟨x_1| ⟨x_2|) (⟨x_1| (\cos θ |z_2⟩ − \sin θ |x_2⟩)) = \frac{1}{\sqrt{2}} \sin θ$$

If photon 1 has polarization in the $x$ direction, then it will not be transmitted by a polarizer in the $z$ direction - it will be absorbed. Hence,

$$P_{++}(\hat{a}, \hat{b}) = |⟨EPR| x_1 z'_2⟩|^2 = \frac{1}{2} \sin^2 θ$$

Similarly,

$$P_{+-}(\hat{a}, \hat{b}) = |⟨EPR| z_1 x'_2⟩|^2 = \frac{1}{2} \sin^2 θ$$
$$P_{-+}(\hat{a}, \hat{b}) = |⟨EPR| x_1 x'_2⟩|^2 = \frac{1}{2} \cos^2 θ$$

The correlation coefficient is then

$$C(\hat{a}, \hat{b}) = P_{++}(\hat{a}, \hat{b}) + P_{--}(\hat{a}, \hat{b}) − P_{+-}(\hat{a}, \hat{b}) − P_{-+}(\hat{a}, \hat{b})$$
$$= \cos^2 θ − \sin^2 θ = 2 \cos^2 θ − 1 = \cos 2θ$$
Since the unit vectors \( \hat{a} \) and \( \hat{b} \) are at an angle \( \theta \) with respect to one another, it follows that

\[
\hat{a} \cdot \hat{b} = \cos \theta
\]

and therefore

\[
C(\hat{a}, \hat{b}) = 2\cos^2 \theta - 1 = 2(\hat{a} \cdot \hat{b})^2 - 1
\]

(3) Show that the maximum value of the Bell coefficient is \( 2\sqrt{2} \) according to quantum mechanics

Suppose that the angle between the vectors \( \hat{a}' \) and \( \hat{a} \) is \( x/2 \), between \( \hat{a} \) and \( \hat{b} \) is \( y/2 \) and between \( \hat{b} \) and \( \hat{b}' \) is \( z/2 \). Then the angle between \( \hat{a}' \) and \( \hat{b}' \) is \( (x + y + z)/2 \) and according to quantum mechanics, the Bell coefficient has the form

\[
B = \cos x + \cos y + \cos z - \cos(x + y + z)
\]

This function has extrema when

\[
\frac{\partial B}{\partial x} = -\sin x + \sin(x + y + z) = 0
\]

\[
\frac{\partial B}{\partial y} = -\sin y + \sin(x + y + z) = 0
\]

\[
\frac{\partial B}{\partial z} = -\sin z + \sin(x + y + z) = 0
\]

or

\[
\sin x = \sin y = \sin z = \sin(x + y + z)
\]

This has the solution

\[
x = y = z \quad , \quad 3x = \pi - x \rightarrow x = \pi/4
\]

For this extremum

\[
B = 3\cos \frac{\pi}{4} - \cos \frac{3\pi}{4} = \frac{3}{\sqrt{2}} + \frac{1}{\sqrt{2}} = 2\sqrt{2}
\]

This is a maximum, since at this point

\[
\frac{\partial^2 B}{\partial x^2} = \frac{\partial^2 B}{\partial y^2} = \frac{\partial^2 B}{\partial z^2} = -\cos \frac{\pi}{4} + \cos \frac{3\pi}{4} = -\sqrt{2} < 0
\]

(4) 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?

Let the vector \( \hat{a} \) be at an angle \( \theta_a \) with respect to some direction in the \( xz \) plane, and let \( \hat{b} \) be at an angle \( \theta_b \) with respect to the same direction. Then

\[
C(\hat{a}, \hat{b}) = \cos 2(\theta_a - \theta_b) = \cos 2\theta_a \cos 2\theta_b + \sin 2\theta_a \sin 2\theta_b
\]

\[
= \int d\lambda \rho(\lambda) C(\hat{a}, \lambda) C(\hat{b}, \lambda)
\]

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and with the assignments
\[ \rho(\lambda) = \delta(\lambda + 1) + \delta(\lambda - 1) \]
\[ C(\hat{a}, 1) = \cos 2\theta_a, \quad C(\hat{a}, -1) = \sin 2\theta_a \]
\[ C(\hat{b}, 1) = \cos 2\theta_b, \quad C(\hat{b}, -1) = \sin 2\theta_b \]
we then see that \( \rho(\lambda) \geq 0 \) and
\[ -1 \leq C(\hat{a}, \lambda), C(\hat{b}, \lambda) \leq 1 \text{ for } \lambda = \pm 1 \]
but
\[ -1 \leq C(\hat{a}, \lambda), C(\hat{b}, \lambda) \leq 1 \text{ for } \lambda = \pm 1 \]
so that the normalization condition (b) 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 \( \theta \), the angle between \( a \) and \( b \).

We let \( |z \pm (\theta)\rangle \) be states corresponding to spin up(down), with respect to a direction at an angle \( \theta \) to the \( z \)-axis. We can write these states (in the \( |z \pm (0)\rangle \) basis) as
\[
|z + (\theta)\rangle = \left( \frac{\cos \frac{1}{2}\theta}{\sin \frac{1}{2}\theta} \right) = \cos \frac{1}{2}\theta \left( \begin{array}{c} 1 \\ 0 \end{array} \right) + \sin \frac{1}{2}\theta \left( \begin{array}{c} 0 \\ 1 \end{array} \right) = \cos \frac{1}{2}\theta |z+\rangle + \sin \frac{1}{2}\theta |z-\rangle \\
|z - (\theta)\rangle = \left( \frac{\sin \frac{1}{2}\theta}{-\cos \frac{1}{2}\theta} \right) = \sin \frac{1}{2}\theta \left( \begin{array}{c} 1 \\ 0 \end{array} \right) - \cos \frac{1}{2}\theta \left( \begin{array}{c} 0 \\ 1 \end{array} \right) = \sin \frac{1}{2}\theta |z+\rangle - \cos \frac{1}{2}\theta |z-\rangle
\]
The singlet state can be written
\[
|EPR\rangle = \frac{1}{\sqrt{2}} \left( |z+\rangle^a |z-\rangle^b - |z-\rangle^a |z+\rangle^b \right)
\]
so that the probability amplitude associated with a measurement of spin up along the \( z \)-axis at \( a \) and (i) a measurement of spin up at \( b \) along a direction at an angle \( \theta \) to the \( z \)-axis is
\[
\langle EPR | z+\rangle^a |z + (\theta)\rangle^b = \langle EPR | z+\rangle^a \left( \cos \frac{1}{2}\theta |z+\rangle^b + \sin \frac{1}{2}\theta |z-\rangle^b \right) \\
= \left( \frac{1}{\sqrt{2}} \left( |z+\rangle^a \langle z-\rangle^b - |z-\rangle^a \langle z+\rangle^b \right) \right) \left( \cos \frac{1}{2}\theta |z+\rangle^a |z+\rangle^b + \sin \frac{1}{2}\theta |z+\rangle^a |z-\rangle^b \right) \\
= \frac{1}{\sqrt{2}} \sin \frac{1}{2}\theta
\]
or (ii) a measurement of spin down at \( b \) along a direction at an angle \( \theta \) to the \( z \)-axis is

\[
\langle EPR \mid z^+ \rangle^a \langle z-(\theta) \rangle^b = \langle EPR \mid z^+ \rangle^a \left( \sin \frac{1}{2} \theta \mid z^+ \rangle^b - \cos \frac{1}{2} \theta \mid z^- \rangle^b \right)
\]

\[
= \left( \frac{1}{\sqrt{2}} \left( \langle z^+ \rangle^a \langle z^+_b - \langle z^- \rangle^a \langle z^+ \rangle^b \right) \left( \sin \frac{1}{2} \theta \langle z^+ \rangle^a \langle z^+ \rangle^b - \cos \frac{1}{2} \theta \langle z^+ \rangle^a \langle z^- \rangle^b \right) \right)
\]

\[
= -\frac{1}{\sqrt{2}} \cos \frac{1}{2} \theta
\]

Therefore, quantum mechanics predicts for the relative frequencies of the coincidences

\[
R(up, up) = \frac{1}{2} \sin^2 \frac{\theta}{2}, \quad R(up, down) = \frac{1}{2} \cos^2 \frac{\theta}{2}
\]

By similar reasoning we find that

\[
R(down, down) = \frac{1}{2} \sin^2 \frac{\theta}{2}, \quad R(down, up) = \frac{1}{2} \cos^2 \frac{\theta}{2}\]

(b) Calculate the correlation coefficient

\[
C(a, b) = R(up, up) - R(up, down) - R(down, up) + R(down, down)
\]

Therefore, the correlation coefficient is

\[
c(a, b) = \frac{1}{2} \sin^2 \frac{\theta}{2} - \frac{1}{2} \cos^2 \frac{\theta}{2} - \frac{1}{2} \cos^2 \frac{\theta}{2} + \frac{1}{2} \sin^2 \frac{\theta}{2} = -\cos \theta
\]

(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

\[
B = C(a, b) + C(a', b) + C(a', b') - C(a, b')
\]

Let us call the angles between \( a \) and \( b \), \( b \) and \( a' \), and \( a' \) and \( b' \) respectively \( \pi - x \), \( \pi - y \), and \( \pi - z \). The angle between \( a \) and \( b' \) is then \( 3\pi - x - y - z \).

Then we find

\[
B(x, y, z) = \cos x + \cos y + \cos z - \cos(x + y + z)
\]

We need to find the maximum of \( B(x, y, z) \). Clearly there is no way to distinguish \( x, y, z \) so they must all be equal. We then have

\[
B(x) = 3 \cos x - \cos(3x)
\]

We then have

\[
\frac{\partial B}{\partial x} = -3 \sin x + 3 \sin(3x) = 0 \rightarrow \sin x = \sin 3x
\]

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or

\[ 4 \sin^3 x - 2 \sin x = 0 \]

Ignoring the solution \( x = y = z = 0 \), we have

\[ \sin^2 x = \frac{1}{2} \rightarrow \cos x = \frac{1}{\sqrt{2}} \rightarrow x = y = z = \frac{\pi}{4} \]

so that the maximum value of \( B(x, y, z) \) is

\[ B(\pi/4) = 3 \cos \pi/4 - \cos(3\pi/4) = \frac{3}{2} \sqrt{2} + \frac{1}{2} \sqrt{2} = 2 \sqrt{2} \]

(d) Show that this prediction of quantum mechanics is inconsistent with classical local realism.

The prediction of quantum mechanics is inconsistent with classical local realism, as can be seen by the method used in problem 16.10.2. Just as in the case for an entangled state of photons, here also the assumption of the existence of local hidden variable, and of separability of the joint conditional probabilities, leads to the Bell inequality, \(|B| \leq 2\), which is violated by quantum mechanics as shown above (part (c)).

16.10.4 Greenberger-Horne-Zeilinger State

The Greenberger-Horne-Zeilinger (GHZ) state of three identical spin–1/2 particles is defined by

\[ |GHZ\rangle = \frac{1}{\sqrt{2}} (|z_a+\rangle |z_b+\rangle |z_c+\rangle - |z_a-\rangle |z_b-\rangle |z_c-\rangle) \]

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 −\( \hbar^3/8 \)

The spin operator, \( \vec{S} \), of an electron can be represented by \( \frac{1}{\hbar} \vec{\sigma} \) where the Cartesian components of \( \vec{\sigma} \) are the Pauli spin matrices. Normalized eigenvectors of the matrices \( \sigma_x \), \( \sigma_y \) and \( \sigma_z \) belonging to eigenvalues +1 and -1, respectively, are

\[
\begin{align*}
|x+\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, & |x-\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\
|y+\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, & |y-\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \\
|z+\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & |z-\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}
\end{align*}
\]
We have the following relations between these eigenvectors:

\[ |z+\rangle = \frac{1}{\sqrt{2}} (|x+\rangle + |x-\rangle) = \frac{1}{\sqrt{2}} (|y+\rangle + |y-\rangle) \]
\[ |z-\rangle = \frac{1}{\sqrt{2}} (|x+\rangle - |x-\rangle) = -\frac{i}{\sqrt{2}} (|y+\rangle - |y-\rangle) \]

Therefore, the GHZ vector can be written in the following five ways:

\[ |GHZ\rangle = \frac{1}{\sqrt{2}} (|z_a+\rangle |z_b+\rangle |z_c+\rangle - |z_a-\rangle |z_b-\rangle |z_c-\rangle) \]
\[ = \frac{1}{\sqrt{2}} (|x_a+\rangle |x_b+\rangle |x_c-\rangle + |x_a-\rangle |x_b+\rangle |x_c+\rangle + |x_a+\rangle |x_b-\rangle |x_c-\rangle + |x_a-\rangle |x_b-\rangle |x_c+\rangle) \]
\[ = \frac{1}{\sqrt{2}} (|y_a+\rangle |y_b-\rangle |y_c-\rangle + |x_a-\rangle |y_b+\rangle |y_c-\rangle + |x_a-\rangle |y_b-\rangle |y_c+\rangle + |x_a+\rangle |y_b-\rangle |y_c+\rangle) \]
\[ = \frac{1}{\sqrt{2}} (|y_a-\rangle |y_b-\rangle |x_c-\rangle + |y_a-\rangle |y_b+\rangle |x_c-\rangle + |y_a-\rangle |y_b-\rangle |x_c+\rangle + |y_a+\rangle |y_b+\rangle |x_c+\rangle) \]
\[ = \frac{1}{\sqrt{2}} (|y_a+\rangle |y_b-\rangle |x_c+\rangle + |y_a-\rangle |y_b+\rangle |x_c+\rangle + |y_a-\rangle |y_b-\rangle |x_c-\rangle + |y_a+\rangle |y_b+\rangle |x_c-\rangle) \]

It follows then that (equation (A))

\[ |GHZ\rangle = -\sigma_a^x \sigma_b^y \sigma_c^x |GHZ\rangle \]
\[ = \sigma_a^x \sigma_b^y \sigma_c^x |GHZ\rangle = \sigma_b^y \sigma_a^x \sigma_c^x |GHZ\rangle = \sigma_c^x \sigma_b^y \sigma_a^x |GHZ\rangle \]

From the first line of (A) we see that the GHZ state is an eigenvector of the product of three \( \sigma_x \) Pauli matrices, \( \sigma_a^x \sigma_b^x \sigma_c^x \) belonging to eigenvalue -1. Since the \( x-\) component of spin is represented by \( \frac{1}{2} \hbar \sigma_x \), it follows that a measurement of the product of three spins in the \( x-\) direction is certainly \( -\frac{1}{2} \hbar^3 \)

(b) the product of two spins in the \( y-\) direction and one spin in the \( x-\) direction is always \( +\hbar^3/8 \)

From the second line of (A) we see that the GHZ state is an eigenvector of the product of one \( \sigma_x \) and two \( \sigma_y \) Pauli matrices, \( \sigma_a^x \sigma_b^y \sigma_c^y \) belonging to eigenvalue +1. It follows that a measurement of the two spins in the \( y-\) direction and one in the \( x-\) direction is certainly \( +\frac{1}{2} \hbar^3 \).

(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

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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

What is the best strategy upon which the players might agree?

Let \( A(X) \) be the agreed answer that A will give if asked the X question, and \( A(Y) \) the agreed answer if she is instead asked the Y question. We define \( B(X) \), \( B(Y) \), \( C(X) \), and \( C(Y) \) similarly. We note that we do not restrict our proof of impossibility to the symmetric situation in which \( A \), \( B \), and \( C \) necessarily give the same answers as each other in the case that they are asked the same question. In order to guarantee success when all players are asked the X question, we need

\[
A(C)B(X)C(X) = -1
\]

If, however, \( A \) is asked X, \( B \) and \( C \) are asked Y, then we need

\[
A(X)B(Y)C(Y) = +1
\]

In the same way, if \( B \) is asked X, but \( A \) and \( C \) are asked Y, we need

\[
A(Y)B(X)C(Y) = +1
\]

and finally, if \( A \) and \( B \) are asked Y, but \( C \) is asked X, then we need

\[
A(Y)B(Y)C(X) = +1
\]

In order to be sure of winning, the team needs all of the above four equations to hold, so that a winning combination of answers is given, no matter which permutation of questions is asked.

To see that these questions are not mutually consistent, multiply all the left hand sides together and equate the answer to the product of the right hand sides, which is clearly −1. However, the product of the left hand sides contains each of the assignments

\[
A(X), A(Y), B(X), B(Y), C(X), C(Y)
\]

twice, that is, every possible assignment occurs as its square. Since each assignment is +1 or −1, the square is in all cases +1, and so the product of all of the left hand sides is +1, contradicting the fact that the product of the right hand sides is −1.
(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

The quantum strategy consists in NOT deciding in advance on the various assignments \( A(X), A(Y), B(X), B(Y), C(X), C(Y) \), but rather in agreeing on the measurement procedure, the precise nature of which depends on whether the \( X \) or the \( Y \) question is asked. On being separated, each player takes with her one of the three electrons that have been prepared in the GHZ state.

They all know what the \( x-\), \( y-\), and \( z-\) directions are, and each player has an apparatus that can measure whether the spin of the electron is ‘up’ or ‘down’ with respect to any of these directions.

If a player is asked the \( X \) question, she orients her apparatus in the \( x-\) direction and makes a spin measurement. If she finds the \( x-\) component of spin is ‘up’, then she gives the answer +1, and if it is ‘down’, she says −1. However, if she is asked then \( Y \) question, then she orients her apparatus in the \( y-\) direction before making her spin measurement. In this case, her answer, +1 or −1, is conditioned by the result of the \( y \) spin measurement.

Here, the classical impossibility proof has been evaded by the expedient of allowing the answers to depend on the results of three measurement, results that are individually indeterminate, but which are correlated in such a way that the game can certainly be won on every playing (100% probability of success).
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

$$H(q, p) = \frac{1}{2m} \left( \vec{p}^2 - \frac{e}{c} \vec{A}(\vec{r}) \right)^2$$

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 \( \mathbf{r}(t) \) of the particle, for the transition amplitude of the process in which the particle returns to its initial location \( \mathbf{r}_0 \) at time \( t_f \) having left that point at \( t_i \), i.e.,

\[
\langle \mathbf{r}_0, t_f | \mathbf{r}_0, t_i \rangle
\]

where \( \mathbf{r}_0 \) 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 \( \mathbf{r}(t) \)?

17.7.2 Path integral for the three-dimensional harmonic oscillator

Consider a harmonic oscillator of mass \( m \) and frequency \( \omega \) in three dimensions. We will denote the position vector of the oscillator by \( \mathbf{r} = (x, y, z) \). The classical Hamiltonian is

\[
H(\mathbf{r}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2 \mathbf{r}^2
\]

Derive an expression for the path integral for the matrix element

\[
\langle \mathbf{r}_f = 0, t_f | \mathbf{r}_i = 0, t_i \rangle
\]

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 \( \omega \), 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 \( W, \tau, m \) and \( \omega \)? Give a physical interpretation to this dependence by looking at the extreme regimes of \( \tau \) 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

\[
\left[i\hbar \partial_t - \hat{H}\right] G(\vec{r}, t; \vec{r}', t') = i\hbar \delta(t - t') \delta(\vec{r} - \vec{r}')
\]

Find explicitly the expression for the green’s function, \(G(t - t', \vec{r} - \vec{r}')\), 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, \(G(\epsilon, \vec{p})\), \((\epsilon \rightarrow \epsilon + i\theta)\) 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](image)

(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.
(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 \( E = \frac{\hbar^2 k^2}{2m_e} \). 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, $D^{(n)}(E)$, for each of the four lowest bands individually. Sketch $D(E)$ 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, $D^{(n)}(E)$, for each of the five lowest bands individually and $D(E)$ for the total of the five lowest bands. Do so in
both the free-electron and weak-binding approximations. Assume all de-
generacies 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 $\eta$ 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:

$$\hat{b}_k = \cosh 2\theta_k \hat{\alpha}_k + \sinh 2\theta_k \hat{\alpha}_k^- , \quad \hat{b}_k^+ = \cosh 2\theta_k \hat{\alpha}_k^+ + \sinh 2\theta_k \hat{\alpha}_{-k}$$

(a) Assume that $E(k), A(k), \theta_k$ 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 $\cosh \theta_k \rightarrow \cos \theta_k$ and $\sinh \theta_k \rightarrow \sin \theta_k$ 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

$$\hat{H} = \sum_k \varepsilon(k)\hat{\alpha}_k^+\hat{\alpha}_k + \frac{1}{2V} \sum_q V_q \sum_{p+k} \hat{\alpha}_p^+\hat{\alpha}_{q+k-p-q}\hat{\alpha}_k\hat{\alpha}_p$$
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.,

\[
\frac{\partial \hat{K}_{cl}}{\partial N_0} \bigg|_{\mu} = 0
\]

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,

\[
\hat{K}_Q = \sum_k \hat{c}_k^+ \hat{c}_k \Omega(k) + K_0
\]

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

\[
\hat{c}_k = \hat{b}_k \cosh \phi_k - \hat{b}_k^- \sinh \phi_k
\]

where \( \hat{b}_k = \hat{b}_k e^{-i\theta} \). Use

\[
e^A Be^{-A} = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \ldots.
\]

to show that

\[
\hat{c}_k = U(\phi) \hat{b}_k U^{-1}(\phi)
\]

where \( U(\phi) \) is the unitary operator

\[
U(\phi) = e^{\sum_k \phi_k (\hat{b}_k^+ \hat{b}_k - \hat{b}_k \hat{b}_k^-)}
\]
(b) Show that the ground state of \( \hat{K} \) in the Bogoliubov approximation is
\[
|GS\rangle = U(\phi) |\tilde{0}\rangle
\]
where \( |\tilde{0}\rangle \) is the vacuum of the operators \( \tilde{b}_k : \tilde{b}_k |\tilde{0}\rangle = 0 \) 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 \( \hat{H} \):
\[
\hat{H} = \int d^3 x \hat{\psi}^+(\vec{x}) \left( -\frac{\hbar^2 \nabla^2}{2m} + U(\vec{x}) \right) \hat{\psi}(\vec{x}) + \frac{1}{2} \int d^3 x d^3 y \hat{\psi}^+(\vec{x}) \hat{\psi}^+(\vec{y}) V(\vec{x} - \vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x})
\]

(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 \( \int |\psi(\vec{x})|^2 d^3 x = N \).

(b) Define new operators \( \hat{\psi}(\vec{x}) \to \psi(\vec{x}) + \eta(\vec{x}) \) where \( \psi(\vec{x}) \) is the solution to the Gross-Pitaevskii equation and write \( \hat{K} \) up to quadratic order in \( \eta(\vec{x}), \eta^+(\vec{x}) \). Show that terms linear in \( \eta(\vec{x}), \eta^+(\vec{x}) \) are cancelled by \( \psi(\vec{x}) \) being a solution to the Gross-Pitaevskii equation.

(c) Introduce the Bogoliubov transformation:
\[
\hat{\phi}(\vec{x}) = u(\vec{x}) \eta(\vec{x}) + v(\vec{x}) \eta^+(\vec{x}) , \quad \hat{\phi}^+(\vec{x}) = u^*(\vec{x}) \eta^+(\vec{x}) + v^*(\vec{x}) \eta(\vec{x})
\]

Show that \( [\hat{\phi}(\vec{x}), \hat{\phi}^+(\vec{y})] = \delta^3(\vec{x} - \vec{y}) \) if \( |u(\vec{x})|^2 + |v(\vec{x})|^2 = 1 \).

(d) Write \( \hat{K} \) up to quadratic order in \( \eta, \eta^+ \) 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

\[ \hat{H} = \int d^3x \, \hat{\psi}^+ \hat{\psi}(\vec{x}) \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\psi}(\vec{x}) + \int d^3x \, d^3y \, \hat{\psi}^+ (\vec{x}) \hat{\psi}^+ (\vec{y}) V(\vec{x} - \vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x}) \]

(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

\[ V(\vec{x} - \vec{y}) = -\frac{e^2}{|\vec{x} - \vec{y}|} \] (19.-18)

which is the Coulomb potential. Namely, consider a weakly interacting Bose gas 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

\[ \hat{K} = \hat{H} - \mu \hat{N} = \sum_k \varepsilon(k) \left( \hat{a}^+_k \hat{a}^+_k \hat{a}^+_{k \uparrow} \hat{a}^+_{k \downarrow} \right) + \sum_k \left[ \Delta \hat{a}^+_k \hat{a}^+_{-k \downarrow} \hat{a}^+_{k \uparrow} + \Delta^* \hat{a}^+_{-k \uparrow} \hat{a}^+_{k \downarrow} \right] \]

where \( \hat{a}^+_k \) are creation operators of an electron of spin up or down and momentum \( \vec{k} \) and

\[ \Delta = -\frac{g}{V} \sum_{k' \neq k} \langle GS | \hat{a}^+_{-k \downarrow} \hat{a}^+_{k \uparrow} | GS \rangle \]

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$|GS\rangle$ is the ground state of $\hat{K}$ and $\sum_{k'}$ is a sum over states with

$$0 \leq \varepsilon(k') \leq \hbar \omega_m$$

and $\varepsilon(k') = \varepsilon(k) - \mu = \frac{k^2 k^2}{2m} - \mu$

(a) Diagonalize $\hat{K}$ by a Bogoliubov transformation, i.e., introduce new operators

$$\hat{A}_k = u_k \hat{a}_k^\uparrow - v_k \hat{a}_{k+1}^\downarrow, \quad \hat{B}_k = v_k \hat{a}_k^\uparrow + u_k \hat{a}_{k+1}^\downarrow$$

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

$$u_k = \left[\frac{1}{2}(1 + \alpha_k)\right]^{1/2}, \quad v_k = -\left[\frac{1}{2}(1 - \alpha_k)\right]^{1/2}$$

Invert the Bogoliubov transformation and write $\hat{K}$ in terms of $\hat{A}, \hat{A}^+, \hat{B}, \hat{B}^+$. Choose $\alpha_k$ so that $\hat{K}$ becomes

$$\hat{K} = \sum_k E(k) \left[\hat{A}_k^+ \hat{A}_k + \hat{B}_k^+ \hat{B}_k\right] + K_0$$

that is, choose $\alpha_k$ to make terms like $\hat{A}\hat{B}$ vanish. Find $E(k)$.

(b) Obtain a self-consistent equation for $\Delta$ by evaluating $\langle GS| \hat{a}_{-k\downarrow} \hat{a}_{k\uparrow} |GS\rangle$ and solve this equation by replacing

$$\frac{1}{V} \sum_{k'} \int_0^{\hbar \omega_m} N(\varepsilon) d\varepsilon$$

where $N(\varepsilon)$ is the density of states so that

$$N(\varepsilon) d\varepsilon = \frac{d^3k}{(2\pi)^3}$$

and assume that $N(\varepsilon) \approx N(0)$.

(c) Obtain the distribution function $\langle GS| \hat{a}_{k\uparrow} \hat{a}_{k\downarrow} |GS\rangle$

(d) Show that $E(0) = \Delta = \text{gap}$ and evaluate the resulting integral in part (b) to give the gap $\Delta$ 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 $\gamma$:

$$H_{ph} = \sum_{n=-\infty}^{\infty} \left[\frac{p_n^2}{2m} + \frac{\gamma}{2}(u_n - u_{n+1})^2\right]$$
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:

$$\hat{u}_k = \sqrt{\frac{\hbar}{2m\omega(k)}}(\hat{a}_k + \hat{a}_k^+), \quad \hat{p}_k = -i\sqrt{\frac{\hbar m\omega(k)}{2}}(\hat{a}_k - \hat{a}_k^+)$$

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 $\gamma'$, so the Hamiltonian of the system has the additional term

$$H'_{ph} = \sum_{n=-\infty}^{\infty} \gamma'(u_n - u_{n+1})^3$$

Rewrite the Hamiltonian in terms of the phonon operators $\hat{a}_k^+$ and $\hat{a}_k$ introduced in part (1). What can you say about momentum conservation of the phonons in the new Hamiltonian?

3. **Electron-Phonon Interaction**

Suppose electrons are also present on the same chain of atoms. Suppose that the electrons can make transitions between neighboring lattice sites with the probability amplitude $t_n$ so that

$$H_{el} = \sum_{n=-\infty}^{\infty} t_n \hat{\psi}_{n+1}^+ \hat{\psi}_n + h.c.$$  

where $\hat{\psi}_n^+$ and $\hat{\psi}_n$ are the fermion operators creating and annihilating electrons on the site $n$.

In the case $t_n = t = \text{constant}$, diagonalize the electron Hamiltonian by Fourier transform $\hat{\psi}_n \to \psi_k$, and determine the spectrum $\varepsilon(k)$ of electronic excitations.

In general, the amplitude of electron tunneling $t_n$ depends on the relative displacement 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 $x^2_{tot}$ in terms of boson operators and taking the expectation value with respect to the ground state of $H_{SB \text{coll}}$.

(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 $E = \sqrt{\vec{p}^2 + m^2}$)

$$u(p, s) = \frac{\vec{p} + m}{\sqrt{E + m}} \begin{pmatrix} \varphi_s \\ 0 \end{pmatrix}, \quad v(p, s) = \frac{-\vec{p} + m}{\sqrt{E + m}} \begin{pmatrix} 0 \\ \chi_s \end{pmatrix}$$

where $\varphi = \gamma^\mu p_\mu$, $\varphi_s (s = \pm 1/2)$ are orthonormalized 2-spinors and similarly for $\chi_s$. 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) $\sum_s u(p, s)\bar{u}(p, s) = \varphi + m$

(e) $\sum_s v(p, s)\bar{v}(p, s) = \varphi - m$

(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 $4 \times 4$ matrix.

(a) Show that the Dirac equation is invariant in form, i.e., $(i\gamma^\mu \partial'_\mu - m) \psi'(x') = 0$, provided

$$S^{-1}(\Lambda)\gamma^\mu S(\Lambda) = \Lambda^\mu_\nu \gamma^\nu$$
(b) For an infinitesimal transformation $\Lambda^\mu_\nu = g^\mu_\nu + \delta\omega^\mu_\nu$, where $\delta\omega^\mu_\nu = -\delta\omega^\nu_\mu$. The spin dependence of $S(\Lambda)$ is given by $I - i\sigma^\mu_\nu\delta\omega^\mu_\nu/4$. Show that $\sigma^\mu_\nu = i[\gamma^\mu, \gamma^\nu]$ satisfies the equation in part (a). For finite transformations we then have $S(\Lambda) = e^{-i\sigma^\mu_\nu\omega^\mu_\nu/4}$.

### 20.8.3 Dirac Equation in 1 + 1 Dimensions

Consider the Dirac equation in 1 + 1 Dimensions (i.e., one space and one time dimension):

$$
\left( i\gamma^0 \frac{\partial}{\partial x^0} + i\gamma^1 \frac{\partial}{\partial x^1} - m \right) \psi(x) = 0
$$

(a) Find a $2 \times 2$ matrix representation of $\gamma^0$ and $\gamma^1$ which satisfies $\{\gamma^\mu, \gamma^\nu\} = 2g^\mu_\nu$ and has correct hermiticity. What is the physical reason that $\psi$ can have only two components in 1 + 1 dimensions?

(b) Find the representation of $\gamma^5 = \gamma^0\gamma^1\gamma^2\gamma^3$, $\sigma^\mu_\nu$ 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 $\psi_+ (x) = u(p^1)e^{-ip^x}$ and $\psi_- (x) = v(p^1)e^{ip^x}$ 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
\[
\gamma^0 = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix}, \quad \gamma = \begin{pmatrix} 0 & \sigma \\ -\sigma & 0 \end{pmatrix}
\]
we have
\[
\psi = \begin{pmatrix} \phi_R \\ \phi_L \end{pmatrix} e^{-i\mathbf{p} \cdot \mathbf{x}}
\]
i.e., that the lower (upper) two components of \(\psi_R (\psi_L)\) vanish.

(b) For the free Dirac equation \((A^\mu = 0)\) show that \(\phi_R\) and \(\phi_L\) are eigenstates of the helicity operator \(\frac{1}{2}\sigma \cdot \mathbf{p}\) with positive and negative helicity, respectively, for plane wave states with \(\mathbf{p}^0 > 0\).

20.8.6 Gyromagnetic Ratio for the Electron
(a) Reduce the Dirac equation \((i\partial - eA - m)\psi = 0\) by multiplying it with \((i\partial - eA + m)\psi = 0\) to the form
\[
\left[(i\partial - eA)^2 - \frac{e}{2}\sigma^{\mu\nu} F_{\mu\nu} - m^2\right] \psi = 0
\]
where \(\sigma^{\mu\nu} = \frac{i}{2} [\gamma^\mu, \gamma^\nu]\) and the field strength \(F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu\).

(b) Show that the dependence in the magnetic field \(B = \nabla \times A\) in the spin-dependent term \(\sigma^{\mu\nu} F_{\mu\nu}\) is of the form \(-\frac{ge}{2m}\Sigma \cdot B\) when the kinetic energy is normalized to \(-\nabla^2/2m\) \((\Sigma = \gamma_5 \gamma^0 \gamma\) is the spin matrix). Determine the value of the gyromagnetic ration \(g\) for the electron.

20.8.7 Dirac \(\rightarrow\) Schrodinger
Reduce the Dirac equation \((i\partial - eA - m)\psi = 0\) for the Hydrogen atom \((A^0 = -Ze/4\pi r, A = 0)\) to the standard Schrodinger equation
\[
i\frac{\partial}{\partial t} \Psi(t, x) = \left(-\frac{\nabla^2}{2m} + eA^0\right) \Psi(t, x)
\]
in the non-relativistic limit, where \(|\mathbf{p}|, A^0 \ll m\). HINT: You may start from the reduced form of the Dirac equation in Problem 20.6(a). Extract the leading time dependence by writing \(\psi(x) = \Psi(t, x)e^{-imt}\).

20.8.8 Positive and Negative Energy Solutions
Positive energy solutions of the Dirac equation correspond to the 4-vector current \(J^\mu = 2p^\mu = 2(E, \mathbf{p}), E > 0\). Show that the negative energy solutions correspond to the current \(J^\mu = -2(E, -\mathbf{p}) = -2(|E|, -\mathbf{p}) = -2p^\mu, E < 0\).
20.8.9 Helicity Operator

(1) Show that the helicity operator commutes with the Hamiltonian:

$$\left[ \vec{\Sigma} \cdot \vec{p}, H \right] = 0$$

(2) Show explicitly that the solutions to the Dirac equation are eigenvectors of the helicity operator:

$$\left[ \vec{\Sigma} \cdot \vec{p} \right] \Psi = \pm \Psi$$

20.8.10 Non-Relativistic Limit

Consider

$$\Psi = \begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

to be a solution of the Dirac equation where $u_A$ and $u_B$ are two-component spinors. Show that in the non-relativistic limit $u_B \sim \beta = v/c$.

20.8.11 Gyromagnetic Ratio

Show that in the non-relativistic 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

$$\left[ \left( \vec{p} - e\vec{A} \right)^2 - \frac{e}{2m} \vec{\sigma} \cdot \vec{B} + eA^0 \right] \chi = E\chi$$

where $\vec{B}$ is the magnetic field, $\sigma^i$ are the Pauli matrices and $E = p^0 - m$. Identify the $g$-factor of the fermion and show that the Dirac equation predicts the correct gyromagnetic ratio for the fermion. To write down the Dirac equation in the presence of an electromagnetic field substitute: $p^\mu \rightarrow p^\mu - eA^\mu$.

20.8.12 Properties of $\gamma_5$

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) $\bar{\Psi}\gamma^\mu\Psi\bar{\Psi}\gamma_5\Psi$

(b) $\bar{\Psi}\gamma_5\Psi\bar{\Psi}\gamma_5\Psi$
20.8.14 A Commutator

Explicitly evaluate the commutator of the Dirac Hamiltonian with the orbital angular momentum operator $\hat{L}$ for a free particle.

20.8.15 Solutions of the Klein-Gordon equation

Let $\phi(\vec{r}, t)$ be a solution of the free Klein-Gordon equation. Let us write

$$\phi(\vec{r}, t) = \psi(\vec{r}, t)e^{-imc^2t/\hbar}$$

Under what conditions will $\psi(\vec{r}, t)$ be a solution of the non-relativistic Schrödinger equation? Interpret your condition physically when $\phi$ is given by a plane-wave solution.

20.8.16 Matrix Representation of Dirac Matrices

The Dirac matrices must satisfy the anti-commutator relationships:

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \quad , \quad \{\alpha_i, \beta\} = 0 \text{ with } \beta^2 = 1$$

(1) Show that the $\alpha_i$, $\beta$ are Hermitian, traceless matrices with eigenvalues $\pm 1$ and even dimensionality.

(2) Show that, as long as the mass term $m$ is not zero and the matrix $\beta$ is needed, there is no $2 \times 2$ set of matrices that satisfy all the above relationships. Hence the Dirac matrices must be of dimension 4 or higher. First show that the set of matrices $\{I, \vec{\sigma}\}$ can be used to express any $2 \times 2$ matrix, i.e., the coefficients $c_0$, $c_i$ always exist such that any $2 \times 2$ 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 $\alpha_i$ in terms of the Pauli matrices, for example $\alpha_i = \sigma_i$ which automatically obeys $\{\alpha_i, \alpha_j\} = 2\delta_{ij}$, and express $\beta$ in terms of $\{I, \vec{\sigma}\}$ using the relation above. Show then that there is no $2 \times 2$ $\beta$ matrix that satisfies $\{\alpha, \beta\} = 0$. 

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20.8.17 Weyl Representation

(1) Show that the Weyl matrices:

\[ \tilde{\alpha} = \begin{pmatrix} -\sigma & 0 \\ 0 & \sigma \end{pmatrix}, \quad \beta = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \]

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

\[ \tilde{\gamma} = \begin{pmatrix} 0 & \sigma \\ -\sigma & 0 \end{pmatrix}, \quad \gamma^0 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \]

(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 \([\tilde{\alpha} \cdot \vec{p} + \beta m] \Psi = E \Psi\) 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

\[ H = \tilde{\alpha} \cdot \vec{p} + \beta m \]

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 \( \sigma^i \sigma^j = \delta^{ij} + i\varepsilon^{ijk} \sigma^k \).
The Dirac equation for a free particle is

\[ i\hbar \frac{\partial |\psi\rangle}{\partial t} = \left( c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc^2 \right) |\psi\rangle \]

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.