Quantum Theory

Problems and Solutions

John R. Boccio
Professor of Physics
Swarthmore College

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2.22.1 Simple Basis Vectors

Given two vectors

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

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

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

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

$$\hat{e}_q \cdot \hat{e}_p = \left(\frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2\right) \cdot \left(-\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2\right) = \frac{1}{2}\left(-\frac{\sqrt{3}}{2}\right) + \frac{\sqrt{3}}{2}\frac{1}{2} = 0$$

so they are orthogonal.

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

$$\begin{aligned}
A_q &= \hat{e}_q \cdot \vec{A} = \left(\tfrac{1}{2}\hat{e}_1 + \tfrac{\sqrt{3}}{2}\hat{e}_2\right)(7\hat{e}_1 + 6\hat{e}_2) = \tfrac{7}{2} + 3\sqrt{3} \\
A_p &= \hat{e}_p \cdot \vec{A} = \left(-\tfrac{\sqrt{3}}{2}\hat{e}_1 + \tfrac{1}{2}\hat{e}_2\right)(7\hat{e}_1 + 6\hat{e}_2) = 3 - \tfrac{7\sqrt{3}}{2} \\
\vec{B}_q &= \hat{e}_q \cdot \vec{B} = \left(\tfrac{1}{2}\hat{e}_1 + \tfrac{\sqrt{3}}{2}\hat{e}_2\right)(-2\hat{e}_1 + 16\hat{e}_2) = 1 + 8\sqrt{3} \\
B_p &= \hat{e}_p \cdot \vec{B} = \left(-\tfrac{\sqrt{3}}{2}\hat{e}_1 + \tfrac{1}{2}\hat{e}_2\right)(-2\hat{e}_1 + 16\hat{e}_2) = \sqrt{3} + 8
\end{aligned}$$

2.22.2 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

$$\begin{aligned} \det\left|A - \lambda I\right| = 0 = &\begin{vmatrix} 1-\lambda & 2 & 4 \\ 2 & 3-\lambda & 0 \\ 5 & 0 & 3-\lambda \end{vmatrix} \\ 0 = &(1-\lambda)(3-\lambda)(3-\lambda) - 20(3-\lambda) - 4(3-\lambda) \\ 0 = &(3-\lambda)(\lambda^2 - 4\lambda - 24) = (3-\lambda)(3+\lambda)(\lambda - 7) \end{aligned}$$

with solutions (eigenvalues)

$$\lambda_1 = 3 \ , \ \lambda_2 = -3 \ , \ \lambda_3 = 7$$

We find the eigenvectors as follows:

$$A\left|1\right\rangle = \lambda_1 \left|1\right\rangle = 3\left|1\right\rangle \quad with \quad \left|1\right\rangle = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

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

$$\begin{aligned} a + 2b + 4c &= 3a \\ 2a + 3b \qquad &= 3b \\ 5a + \qquad 3c &= 3c \end{aligned}$$

which give

$$a = 0 \ , \ b = -2c$$

Since the eigenvector must be normalized to 1 we have

$$a = 0 \ , \ b = -\frac{2}{\sqrt{5}} \ , \ c = \frac{1}{\sqrt{5}} \to \left|1\right\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix}$$

Similarly, we find

$$|2\rangle = \frac{1}{\sqrt{65}}\begin{pmatrix} -6 \\ 2 \\ 5 \end{pmatrix} \quad , \quad |3\rangle = \frac{1}{\sqrt{45}}\begin{pmatrix} 4 \\ 2 \\ 5 \end{pmatrix}$$

We then find that

$$\langle 1 \mid 2\rangle = \frac{1}{\sqrt{325}} \neq 0 \quad , \quad \langle 1 \mid 3\rangle = \frac{1}{\sqrt{225}} \neq 0 \quad , \quad \langle 2 \mid 3\rangle = \frac{1}{\sqrt{117}} \neq 0$$

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

2.22.3 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 eigenvalue 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

$$\begin{pmatrix} 2 & 2 & 0 \\ 1 & 2 & 1 \\ 1 & 2 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0 \Rightarrow \begin{matrix} a+b=0 \\ a+2b+c=0 \\ a^2+b^2+c^2=1 \end{matrix} \Rightarrow \begin{matrix} b=-a \\ c=a \\ 3a^2=1 \end{matrix} \Rightarrow \begin{matrix} a=1/\sqrt{3} \\ b=-1/\sqrt{3} \\ c=1/\sqrt{3} \end{matrix}$$
$$|0\rangle = \tfrac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 2 & 2 & 0 \\ 1 & 2 & 1 \\ 1 & 2 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{matrix} 2a+2b=a \\ a+2b+c=b \\ a^2+b^2+c^2=1 \end{matrix} \Rightarrow \begin{matrix} b=-a/2 \\ c=b \\ 3a^2/2=1 \end{matrix} \Rightarrow \begin{matrix} a=\sqrt{2/3} \\ b=-1/\sqrt{6} \\ c=-1/\sqrt{6} \end{matrix}$$
$$|1\rangle = \tfrac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}$$

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

$$|4\rangle = \tfrac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Gram-Schmidt:

$$|0'\rangle = |0\rangle = \tfrac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$$

$$|1'\rangle = |1\rangle - \tfrac{\langle 1|0'\rangle}{\langle 0'|0'\rangle} |0'\rangle = \tfrac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix} - \tfrac{2}{3\sqrt{2}} \tfrac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = \tfrac{1}{3\sqrt{6}} \begin{pmatrix} 4 \\ -1 \\ -5 \end{pmatrix} \underset{normalizing}{\Rightarrow} \tfrac{1}{\sqrt{42}} \begin{pmatrix} 4 \\ -1 \\ -5 \end{pmatrix}$$

$$|4'\rangle = |4\rangle - \tfrac{\langle 4|0'\rangle}{\langle 0'|0'\rangle} |0'\rangle - \tfrac{\langle 4|1'\rangle}{\langle 1'|1'\rangle} |1'\rangle = \tfrac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \tfrac{1}{3} \tfrac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} - \tfrac{(-2)}{\sqrt{3}\sqrt{42}} \tfrac{1}{\sqrt{42}} \begin{pmatrix} 4 \\ -1 \\ -5 \end{pmatrix}$$

$$= \tfrac{3}{7\sqrt{3}} \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix} \underset{normalizing}{\Rightarrow} \tfrac{1}{\sqrt{14}} \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix}$$

giving the orthonormal set of eigenvectors

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

2.22.4 Operator Matrix Representation

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

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

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

We have

$$\begin{aligned} \langle 1|\hat{G}|1\rangle &= 2\langle 1 \mid 1\rangle - 4\langle 1 \mid 2\rangle + 7\langle 1 \mid 3\rangle = 2 = G_{11} \\ \langle 2|\hat{G}|1\rangle &= 2\langle 2 \mid 1\rangle - 4\langle 2 \mid 2\rangle + 7\langle 2 \mid 3\rangle = -4 = G_{21} \\ \langle 3|\hat{G}|1\rangle &= 2\langle 3 \mid 1\rangle - 4\langle 3 \mid 2\rangle + 7\langle 3 \mid 3\rangle = 7 = G_{31} \\ \langle 1|\hat{G}|2\rangle &= -2\langle 1 \mid 1\rangle + 3\langle 1 \mid 3\rangle = -2 = G_{12} \\ \langle 2|\hat{G}|2\rangle &= -2\langle 2 \mid 1\rangle + 3\langle 2 \mid 3\rangle = 0 = G_{22} \\ \langle 3|\hat{G}|2\rangle &= -2\langle 3 \mid 1\rangle + 3\langle 3 \mid 3\rangle = 3 = G_{32} \\ \langle 1|\hat{G}|3\rangle &= 11\langle 1 \mid 1\rangle + 2\langle 1 \mid 2\rangle - 6\langle 1 \mid 3\rangle = 11 = G_{13} \\ \langle 2|\hat{G}|3\rangle &= 11\langle 2 \mid 1\rangle + 2\langle 2 \mid 2\rangle - 6\langle 2 \mid 3\rangle = 2 = G_{23} \\ \langle 3|\hat{G}|3\rangle &= 11\langle 3 \mid 1\rangle + 2\langle 3 \mid 2\rangle - 6\langle 3 \mid 3\rangle = -6 = G_{33} \end{aligned}$$

so that

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

2.22.5 Matrix Representation and Expectation Value

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

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

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

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

$$\hat{K} = 2|1\rangle\langle 1| + 3|2\rangle\langle 2| - 6|3\rangle\langle 3|$$

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 $\langle\alpha|\hat{K}|\alpha\rangle$, in the state

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

We have

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

and

$$\left\langle \hat{K} \right\rangle = \langle\alpha|\hat{K}|\alpha\rangle = \sum_{n=1}^{3} k_n P(k_n)$$

We will evaluate this in three ways.

Matrix Multiplication:

$$\left\langle \hat{K} \right\rangle = \langle\alpha|\hat{K}|\alpha\rangle = \frac{1}{\sqrt{83}}(-3, 5, 7)\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix}\frac{1}{\sqrt{83}}\begin{pmatrix} -3 \\ 5 \\ 7 \end{pmatrix} = -\frac{201}{83}$$

Bra-Kets:

$$\begin{aligned}\left\langle \hat{K} \right\rangle &= \tfrac{1}{\sqrt{83}}\left(-3\left\langle 1\right| + 5\left\langle 2\right| + 7\left\langle 3\right|\right)\left(2\left|1\right\rangle\left\langle 1\right| + 3\left|2\right\rangle\left\langle 2\right| - 6\left|3\right\rangle\left\langle 3\right|\right)\tfrac{1}{\sqrt{83}}\left(-3\left|1\right\rangle + 5\left|2\right\rangle + 7\left|3\right\rangle\right) \\ &= \tfrac{1}{83}\left(-3\left\langle 1\right| + 5\left\langle 2\right| + 7\left\langle 3\right|\right)\left(-6\left|1\right\rangle + 15\left|2\right\rangle - 42\left|3\right\rangle\right) - \tfrac{201}{83}\end{aligned}$$

Probabilities:

$$\begin{aligned}\left\langle \hat{K} \right\rangle &= \left\langle \alpha\right| \hat{K}\left|\alpha\right\rangle = \sum_{n=1}^{3} k_n P(k_n) = 2\left|\left\langle 1 \mid \alpha\right\rangle\right|^2 + 3\left|\left\langle 2 \mid \alpha\right\rangle\right|^2 - 6\left|\left\langle 3 \mid \alpha\right\rangle\right|^2 \\ &= 2\tfrac{9}{83} + 3\tfrac{25}{83} - 6\tfrac{49}{83} = -\tfrac{201}{83}\end{aligned}$$

2.22.6 Projection Operator Representation

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

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

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

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

$$\left|0\right\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} , \left|2\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} , \left|3\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Finally,

$$\hat{P}_2\left|A\right\rangle = \left|2\right\rangle\left\langle 2 \mid A\right\rangle = \frac{5}{\sqrt{83}}\left|2\right\rangle$$

We also note that

$$\begin{aligned}&\hat{P}_2^2 = (\left|2\right\rangle\left\langle 2\right|)(\left|2\right\rangle\left\langle 2\right|) = \left|2\right\rangle\left\langle 2\right| = \hat{P}_2 \\ &\hat{P}_2^2\left|\lambda\right\rangle = \hat{P}_2\left|\lambda\right\rangle = \lambda\left|\lambda\right\rangle \\ &\qquad = \hat{P}_2(\hat{P}_2\left|\lambda\right\rangle) = \hat{P}_2(\lambda\left|\lambda\right\rangle) = \lambda(\hat{P}_2\left|\lambda\right\rangle) = \lambda^2\left|\lambda\right\rangle\end{aligned}$$

or

$$\begin{aligned}&\lambda^2\left|\lambda\right\rangle = \lambda\left|\lambda\right\rangle \rightarrow (\lambda^2 - \lambda)\left|\lambda\right\rangle = 0 \\ &(\lambda^2 - \lambda) = 0 \rightarrow \lambda = 0, 1\end{aligned}$$

So projection operators are idempotent operators.

2.22.7 Operator Algebra

An operator for a two-state system is given by

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

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

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

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

To find the eigenkets we have

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

which gives

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

so that

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

Normalizing, we have

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

and similarly (or using orthonormality),

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

Since $\langle + \mid -\rangle = 0$, they are orthogonal. We also have

$$|+\rangle\langle +| = \tfrac{1}{1.17}\left(|1\rangle\langle 1| + 0.17|2\rangle\langle 2| + 0.41|1\rangle\langle 2| + 0.41|2\rangle\langle 1|\right)$$
$$|-\rangle\langle -| = \tfrac{1}{6.81}\left(|1\rangle\langle 1| + 5.81|2\rangle\langle 2| - 2.41|1\rangle\langle 2| - 2.41|2\rangle\langle 1|\right)$$

so that

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

as it should.

2.22.8 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

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

Now assume that (induction proof)

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

This implies that

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

We then have

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

2.22.9 A Symmetric Matrix

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

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

Find the matrix A.

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

$$D = UAU^T$$

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

$$A = U^{-1} D \left(U^T\right)^{-1} = U^T D U$$

We thus obtain

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

2.22.10 Determinants and Traces

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

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

Any $n \times n$ matrix can be brought into triangular from 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 (λ_i). Now we have

$$A = R T R^{-1}$$

and therefore

$$\exp A = \exp(RTR^{-1}) = \sum_n \frac{(RTR^{-1})^n}{n!} = R \sum_n \frac{(T)^n}{n!} R^{-1} = R \exp(T) R^{-1}$$

Since T is triangular, the diagonal elements of the k^{th} power of T are λ_i^k where k is a positive integer. Consequently, the diagonal elements of $exp(T)$ are $exp(\lambda_j)$. Since the determinant of a triangular matrix is equal to the product of the diagonal elements, we find

$$\det(\exp(T)) = \exp(\lambda_1 + \lambda_2 + ... + \lambda_n) = \exp(tr(T))$$

Since

$$tr(T) = tr(R^{-1} A R) = tr(A R R^{-1}) = tr(A)$$

and

$$\det(\exp(T)) = \det(\mathrm{R} exp(T) R^{-1}) = \det(exp(\mathrm{R} T R^{-1})) = \det(\exp(A))$$

we get

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

Another solution method:

$$e^{(Tr(A))} = e^{(\sum_n a_n)} = \prod e^{a_n}$$

where the a_n are the eigenvalues of A. From 4.22.8 we have

$$\text{if } A\left|a_n\right\rangle = a_n\left|a_n\right\rangle \text{ then } e^A\left|a_n\right\rangle = e^{a_n}\left|a_n\right\rangle$$

by Taylor expansion. Therefore

$$\det e^A = \prod_n a_n' = \prod_n e^{a_n} = e^{TrA}$$

2.22.11 Function of a Matrix

Let

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

Calculate $\exp(\alpha A)$, α 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

$$e^{\varepsilon D} = \exp(\varepsilon UAU^{-1}) = U\exp(\varepsilon A)U^{-1}$$

Therefore

$$\exp(\varepsilon A) = U^{-1}e^{\varepsilon D}U$$

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

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

2.22.12 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

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

We find

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

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

$$u_1' = u_1 \quad , \quad u_2' = u_2 + \alpha u_1 \quad , \quad u_3' = u_3$$

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.

2.22.13 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

$$\det(AB) = \det(A)\det(B)\ , \ \det(A) = \det(A^T)\ , \ \det(I) = 1$$

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

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

Then the transpose matrix A^T of A is given by

$$A^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \ldots \\ 1 & 0 & 0 & 0 & 0 & \ldots \\ 0 & 1 & 0 & 0 & 0 & \ldots \\ 0 & 0 & 1 & 0 & 0 & . \\ . & . & . & . & . & . \end{pmatrix}$$

It follows that

$$AA^T = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \ldots \\ 0 & 1 & 0 & 0 & 0 & \ldots \\ 0 & 0 & 1 & 0 & 0 & \ldots \\ 0 & 0 & 0 & 1 & 0 & . \\ . & . & . & . & . & . \end{pmatrix} = I$$

and

$$A^T A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & ... \\ 0 & 1 & 0 & 0 & 0 & ... \\ 0 & 0 & 1 & 0 & 0 & ... \\ 0 & 0 & 0 & 1 & 0 & . \\ . & . & . & . & . & . \end{pmatrix} \neq I$$

Consequently,

$$AA^T \neq A^T A$$

2.22.14 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

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

Therefore,

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

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

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

and then we have

$$0\hat{P}_0 + \sqrt{2}\hat{P}_{\sqrt{2}} - \sqrt{2}\hat{P}_{-\sqrt{2}} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} = M$$

2.22.15 Measurement Results

Given particles in state

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

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

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

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

We have

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

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

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

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

$$\begin{aligned}
P(2|\alpha) &= |\langle 1 \mid \alpha\rangle|^2 = \tfrac{1}{83} \left|-3\,\langle 1 \mid 1\rangle + 5\,\langle 1 \mid 2\rangle + 7\,\langle 1 \mid 3\rangle\right|^2 = \tfrac{9}{83} \\
P(3|\alpha) &= |\langle 2 \mid \alpha\rangle|^2 = \tfrac{1}{83} \left|-3\,\langle 2 \mid 1\rangle + 5\,\langle 2 \mid 2\rangle + 7\,\langle 2 \mid 3\rangle\right|^2 = \tfrac{25}{83} \\
P(-6|\alpha) &= |\langle 3 \mid \alpha\rangle|^2 = \tfrac{1}{83} \left|-3\,\langle 3 \mid 1\rangle + 5\,\langle 3 \mid 2\rangle + 7\,\langle 3 \mid 3\rangle\right|^2 = \tfrac{49}{83}
\end{aligned}$$

2.22.16 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 $\left\langle R^2 \right\rangle = \langle\Psi| R^2 |\Psi\rangle$ 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

$$\begin{aligned} \left\langle R^2 \right\rangle = \langle\Psi| R^2 |\psi\rangle &= \begin{bmatrix} a \\ b \end{bmatrix}^+ \begin{bmatrix} 40 & -30 \\ -30 & 85 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = (a^* \; b^*) \begin{bmatrix} 40 & -30 \\ -30 & 85 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \\ &= 40 \left|a\right|^2 + 85 \left|b\right|^2 - 60\text{Real}(a^* b) \end{aligned}$$

(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

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

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

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

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

$$\begin{aligned} \left\langle R^2 \right\rangle = \langle\Psi| R^2 |\Psi\rangle &= (5)^2 P(5) + (10)^2 P(10) = (5)^2 \left|\langle 5 \mid \Psi\rangle\right|^2 + (10)^2 \left|\langle 10 \mid \Psi\rangle\right|^2 \\ &= \tfrac{25}{5} \left|2a + b\right|^2 + \tfrac{100}{5} \left|a - 2b\right|^2 = 40 \left|a\right|^2 + 85 \left|b\right|^2 - 60\text{Real}(a^* b) \end{aligned}$$

as before.

2.22.17 Eigenket Properties

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

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

where a and b are both real numbers.

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

Since $\hat{A}$ is diagonal, its eigenvalues are $a, -a, -a$. For $\hat{B}$, the characteristic equation is

$$\begin{vmatrix} b-\lambda & 0 & 0 \\ 0 & -\lambda & -ib \\ 0 & ib & -\lambda \end{vmatrix} = 0 = \lambda^2(b-\lambda) - b^2(b-\lambda)$$

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

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

(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 $\left|u^i\right\rangle$ be the eigenvector of $\hat{B}$ with eigenvalue λ_i, that is,

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

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

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

We choose the solution

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

For $\lambda_2 = b$ (degenerate eigenvalue) we have the same equations as above and, in addition, must have $\left\langle u^1 \mid u^2 \right\rangle = 0$ (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

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

For the non-degenerate eigenvalue $\lambda_3 = -b$, we must have $\langle u^1 \mid u^3 \rangle = 0 = \langle u^2 \mid u^3 \rangle$ (orthogonal to the other two eigenvectors). If we choose $u_1^3 = 0$ (guarantees $\langle u^1 \mid u^3 \rangle = 0$) and $u_2^3 = 1$, then the equation $ibu_2^3 = -bu_3^3$ says that $u_3^2 = -i$, so that

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

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

2.22.18 The World of Hard/Soft Particles

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

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

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

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

Suppose that we are in the state

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

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

$$\begin{aligned} \langle A \mid A\rangle &= \left(\cos\theta\,\langle h| + e^{-i\varphi}\sin\theta\,\langle s|\right)\left(\cos\theta\,|h\rangle + e^{i\varphi}\sin\theta\,|s\rangle\right) \\ &= \cos^2\theta\,\langle h \mid h\rangle + e^{i\varphi}\sin\theta\cos\theta\,\langle h \mid s\rangle + e^{-i\varphi}\sin\theta\cos\theta\,\langle s \mid h\rangle + \sin^2\theta\,\langle s \mid s\rangle \\ &= \cos^2\theta + \sin^2\theta = 1 \end{aligned}$$

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.

$$\begin{aligned} &|B\rangle = \alpha\,|h\rangle + \beta\,|s\rangle \\ &\langle A \mid B\rangle = \left(\cos\theta\,\langle h| + e^{-i\varphi}\sin\theta\,\langle s|\right)(\alpha\,|h\rangle + \beta\,|s\rangle) = 0 \\ &\quad 0 = \alpha\cos\theta + e^{-i\varphi}\beta\sin\theta \Rightarrow \beta = -e^{i\varphi}\alpha\cot\theta \\ &\langle B \mid B\rangle = (\alpha^*\,\langle h| + \beta^*\,\langle s|)(\alpha\,|h\rangle + \beta\,|s\rangle) = |\alpha|^2 + |\beta|^2 = 1 \\ &|\alpha|^2 + \cot^2\theta\,|\alpha|^2 = 1 \Rightarrow |\alpha|^2 = \tfrac{1}{1+\cot^2\theta} = \sin^2\theta \\ &\alpha = \sin\theta \quad , \quad \beta = -e^{i\varphi}\cos\theta \\ &|B\rangle = \sin\theta\,|h\rangle - e^{i\varphi}\cos\theta\,|s\rangle \end{aligned}$$

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

$$
\begin{aligned}
&|A\rangle = \cos\theta\,|h\rangle + e^{i\varphi}\sin\theta\,|s\rangle \\
&|B\rangle = \sin\theta\,|h\rangle - e^{i\varphi}\cos\theta\,|s\rangle \\
&\langle h \mid A\rangle = \cos\theta = \langle A \mid h\rangle \quad , \quad \langle h \mid B\rangle = \sin\theta = \langle B \mid h\rangle \\
&\langle s \mid A\rangle = e^{i\varphi}\sin\theta = \langle A \mid s\rangle^* \quad , \quad \langle s \mid B\rangle = -e^{i\varphi}\cos\theta = \langle B \mid s\rangle^* \\
&|h\rangle = \langle A \mid h\rangle\,|A\rangle + \langle B \mid h\rangle\,|B\rangle = \cos\theta\,|A\rangle + \sin\theta\,|B\rangle \\
&|s\rangle = \langle A \mid s\rangle\,|A\rangle + \langle B \mid s\rangle\,|B\rangle \\
&\quad = e^{-i\varphi}\sin\theta\,|A\rangle - e^{-i\varphi}\cos\theta\,|B\rangle = e^{-i\varphi}\left(\sin\theta\,|A\rangle - \cos\theta\,|B\rangle\right) \\
&|s\rangle = \sin\theta\,|A\rangle - \cos\theta\,|B\rangle
\end{aligned}
$$

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?

$$
\begin{aligned}
P(h|A) &= |\langle h \mid A\rangle|^2 = \cos^2\theta \\
P(s|A) &= |\langle s \mid A\rangle|^2 = \sin^2\theta
\end{aligned}
$$

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

$$
\begin{aligned}
\hat{H} &= |h\rangle\langle h| - |s\rangle\langle s| \\
H &= \begin{pmatrix} \langle A|\hat{H}|A\rangle & \langle A|\hat{H}|B\rangle \\ \langle B|\hat{H}|A\rangle & \langle B|\hat{H}|B\rangle \end{pmatrix} \\
&= \begin{pmatrix} \langle A \mid h\rangle\langle h \mid A\rangle - \langle A \mid s\rangle\langle s \mid A\rangle & \langle A \mid h\rangle\langle h \mid B\rangle - \langle A \mid s\rangle\langle s \mid B\rangle \\ \langle B \mid h\rangle\langle h \mid A\rangle - \langle B \mid s\rangle\langle s \mid A\rangle & \langle B \mid h\rangle\langle h \mid B\rangle - \langle B \mid s\rangle\langle s \mid B\rangle \end{pmatrix} \\
&= \begin{pmatrix} \cos^2\theta - \sin^2\theta & 2\sin\theta\cos\theta \\ 2\sin\theta\cos\theta & \sin^2\theta - \cos^2\theta \end{pmatrix} = \begin{pmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{pmatrix}
\end{aligned}
$$

or

$$
\begin{aligned}
\hat{H} &= |h\rangle\langle h| - |s\rangle\langle s| \\
&= \left(\cos\theta\,|A\rangle + \sin\theta\,|B\rangle\right)\left(\cos\theta\,\langle A| + \sin\theta\,\langle B|\right) \\
&\qquad - \left(\sin\theta\,|A\rangle - \cos\theta\,|B\rangle\right)\left(\sin\theta\,\langle A| - \cos\theta\,\langle B|\right) \\
&= \cos 2\theta\,|A\rangle\langle A| + \sin 2\theta\,|B\rangle\langle A| + \sin 2\theta\,|A\rangle\langle B| - \cos 2\theta\,|B\rangle\langle B|
\end{aligned}
$$

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

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

so that

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

2.22.19 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

$$\begin{aligned}|\lambda_1\rangle &= |0\rangle \\ |\lambda_1\rangle &= \tfrac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right) \\ |\lambda_2\rangle &= \tfrac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right) \\ |\lambda_3\rangle &= |3\rangle\end{aligned}$$

(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.,

$$\begin{aligned}\hat{B}|\Psi\rangle &= \left(\tfrac{1}{\sqrt{2}}(\hat{I} + |\Psi\rangle\langle\Psi|)\right)|\Psi\rangle = \tfrac{1}{\sqrt{2}}(\hat{I}|\Psi\rangle + |\Psi\rangle\langle\Psi \mid \Psi\rangle) \\ &= \tfrac{2}{\sqrt{2}}|\Psi\rangle = \sqrt{2}|\Psi\rangle\end{aligned}$$

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

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

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.

2.22.20 A 2-Dimensional Hilbert Space

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

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

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

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

and similarly for $\hat{S}_y$ and $\hat{S}_z$.

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

$$\begin{aligned}\left[\hat{S}_x\right] &= \begin{pmatrix} \langle\uparrow|\hat{S}_x|\uparrow\rangle & \langle\uparrow|\hat{S}_x|\downarrow\rangle \\ \langle\downarrow|\hat{S}_x|\uparrow\rangle & \langle\downarrow|\hat{S}_x|\downarrow\rangle \end{pmatrix} \\ &= \tfrac{\hbar}{2}\begin{pmatrix} \langle\uparrow|\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right)|\uparrow\rangle & \langle\uparrow|\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right)|\downarrow\rangle \\ \langle\downarrow|\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right)|\uparrow\rangle & \langle\downarrow|\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right)|\downarrow\rangle \end{pmatrix} = \tfrac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\end{aligned}$$

and similarly,

$$\left[\hat{S}_y\right] = \frac{\hbar}{2i}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \left[\hat{S}_z\right] = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

$$\begin{aligned}\left[\hat{S}_x, \hat{S}_y\right] &= \tfrac{\hbar^2}{4i}\left[\begin{array}{c} \left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right)\left(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|\right) \\ -\left(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|\right)\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right) \end{array}\right] \\ &= \tfrac{\hbar^2}{4i}\left[-|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| - |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right] = i\hbar\hat{S}_z\end{aligned}$$

$$\begin{aligned}\left[\hat{S}_x, \hat{S}_y\right] &= \tfrac{\hbar^2}{4i}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] \\ &= \tfrac{\hbar^2}{4i}\left[\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\right] = i\hbar\tfrac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = i\hbar\hat{S}_z\end{aligned}$$

Now let

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

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

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

$$\begin{aligned}\langle + \mid + \rangle &= \tfrac{1}{2}\left(\langle\uparrow| + |\downarrow\rangle\right)\left(|\uparrow\rangle - |\downarrow\rangle\right) = \tfrac{1}{2}(1+1) = 1 = \langle - \mid - \rangle \\ \langle + \mid - \rangle &= \tfrac{1}{2}\left(\langle\uparrow| + |\downarrow\rangle\right)\left(|\uparrow\rangle - |\downarrow\rangle\right) = \tfrac{1}{2}(1-1) = 0 = \langle - \mid + \rangle\end{aligned}$$

so they form an orthonormal basis.

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

$$\left[\hat{S}_x\right]^{\pm} = \frac{\hbar}{2}\frac{1}{2}\begin{pmatrix} (\langle\uparrow| + \langle\downarrow|)(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)(|\uparrow\rangle + |\downarrow\rangle) & (\langle\uparrow| + \langle\downarrow|)(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)(|\uparrow\rangle - |\downarrow\rangle) \\ (\langle\uparrow| - \langle\downarrow|)(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)(|\uparrow\rangle + |\downarrow\rangle) & (\langle\uparrow| - \langle\downarrow|)(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)(|\uparrow\rangle - |\downarrow\rangle) \end{pmatrix}$$
$$= \frac{\hbar}{4}\begin{pmatrix} 1+1 & -1+1 \\ 1-1 & -1-1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \hat{S}_z$$

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

$$\left[\hat{S}_y\right]^{\pm} = \frac{\hbar}{2}\frac{1}{2i}\begin{pmatrix} (\langle\uparrow| + \langle\downarrow|)(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|)(|\uparrow\rangle + |\downarrow\rangle) & (\langle\uparrow| + \langle\downarrow|)(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|)(|\uparrow\rangle - |\downarrow\rangle) \\ (\langle\uparrow| - \langle\downarrow|)(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|)(|\uparrow\rangle + |\downarrow\rangle) & (\langle\uparrow| - \langle\downarrow|)(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|)(|\uparrow\rangle - |\downarrow\rangle) \end{pmatrix}$$
$$= \frac{\hbar}{4i}\begin{pmatrix} 1-1 & -1-1 \\ 1+1 & -1+1 \end{pmatrix} = \frac{\hbar}{2i}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -\hat{S}_y$$

$$\left[\hat{S}_z\right]^{\pm} = \frac{\hbar}{2}\frac{1}{2}\begin{pmatrix} (\langle\uparrow| + \langle\downarrow|)(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)(|\uparrow\rangle + |\downarrow\rangle) & (\langle\uparrow| + \langle\downarrow|)(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)(|\uparrow\rangle - |\downarrow\rangle) \\ (\langle\uparrow| - \langle\downarrow|)(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)(|\uparrow\rangle + |\downarrow\rangle) & (\langle\uparrow| - \langle\downarrow|)(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)(|\uparrow\rangle - |\downarrow\rangle) \end{pmatrix}$$
$$= \frac{\hbar}{4}\begin{pmatrix} 1-1 & 1+1 \\ 1+1 & 1-1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \hat{S}_x$$

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

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

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

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

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

Therefore, we want

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

and

$$U^\dagger\left[\hat{S}_z\right]^{\pm} U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
$$= \frac{\hbar}{4}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{\hbar}{4}\begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix} = \hat{S}_z$$
$$= \frac{\hbar}{4}\begin{pmatrix} 1+1 & -1+1 \\ 1-1 & -1-1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \hat{S}_z$$

$$U^\dagger\left[\hat{S}_x\right]^{\pm} U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
$$= \frac{\hbar}{4}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \frac{\hbar}{4}\begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix} = \hat{S}_x$$

$$U^\dagger \left[\hat{S}_y\right]^\pm U = -\tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tfrac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
$$= -\tfrac{\hbar i}{4}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} = -\tfrac{\hbar i}{4}\begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix} = -\hat{S}_y$$

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 $\hat{S}_+^\dagger = \hat{S}_-$.

$$\hat{S}_\pm = \tfrac{1}{2}\left(\hat{S}_x \pm i\hat{S}_y\right) = \tfrac{1}{2}\left(\tfrac{\hbar}{2}\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right) \pm i\tfrac{\hbar}{2i}\left(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|\right)\right)$$
$$\hat{S}_+ = \tfrac{\hbar}{2}|\uparrow\rangle\langle\downarrow| \quad , \quad \hat{S}_- = \tfrac{\hbar}{2}|\downarrow\rangle\langle\uparrow|$$

(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

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

$$\hat{S}_+|\downarrow\rangle = \left(\tfrac{\hbar}{2}|\uparrow\rangle\langle\downarrow|\right)|\downarrow\rangle = \tfrac{\hbar}{2}|\uparrow\rangle \quad , \quad \hat{S}_-|\uparrow\rangle = \left(\tfrac{\hbar}{2}|\downarrow\rangle\langle\uparrow|\right)|\uparrow\rangle = \tfrac{\hbar}{2}|\downarrow\rangle$$
$$\hat{S}_+|\uparrow\rangle = \left(\tfrac{\hbar}{2}|\uparrow\rangle\langle\downarrow|\right)|\uparrow\rangle = 0 \quad , \quad \hat{S}_-|\downarrow\rangle = \left(\tfrac{\hbar}{2}|\downarrow\rangle\langle\uparrow|\right)|\downarrow\rangle = 0$$

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

2.22.21 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 (α, 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 $J^2(M^2)$. 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 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 $|\alpha, 0, 0\rangle$ with eigenvalue) of 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:

value	$6\hbar^2$	$15\hbar^2/4$	$2\hbar^2$	$3\hbar^2/4$	0
times	5	32	81	96	42

for a total of 256.

2.22.22 Operator Properties

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

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, $(d/dx)^+$?

We have

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

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, $(AB)^+ = B^+A^+$

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 ψ_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 wrtie

$$\int \psi_3^*\psi_4\, dx = \left(\int \psi_4^*\psi_3\, dx\right)^*$$

(because ψ_3^* and ψ_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 $(AB)^\dagger = B^\dagger A^\dagger$

2.22.23 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

$$\begin{aligned}
\frac{\partial}{\partial t}\langle O\rangle &= \frac{\partial}{\partial t}\langle\psi|\, O\,|\psi\rangle \\
&= \left[\frac{\partial}{\partial t}\langle\psi|\right] O\,|\psi\rangle + \langle\psi|\, O\left[\frac{\partial}{\partial t}|\psi\rangle\right] \\
&= \left[-\langle\psi|\,\frac{1}{i\hbar}H\right] O\,|\psi\rangle + \langle\psi|\, O\left[\frac{1}{i\hbar}H\,|\psi\rangle\right] \\
&= \frac{i}{\hbar}\langle\psi|\,(HO - OH)\,|\psi\rangle
\end{aligned}$$

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:

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

We have

$$\begin{aligned}
\frac{d}{dt}\langle x\rangle &= \frac{i}{\hbar}\langle[H,x]\rangle = \frac{i}{\hbar}\langle\frac{1}{2m}[p_x^2,x]\rangle \\
&= \frac{i}{2m\hbar}\langle(p_xp_xx - xp_xp_x)\rangle = \frac{i}{2m\hbar}\langle(p_xp_xx - p_xxp_x + p_xxp_x - xp_xp_x)\rangle \\
&= \frac{i}{2m\hbar}\langle(p_x[p_x,x] + [p_x,x]p_x)\rangle = \frac{i}{2m\hbar}\langle(-2i\hbar p_x)\rangle \\
&= \langle\frac{p_x}{m}\rangle
\end{aligned}$$

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

$$\begin{aligned}
\frac{d}{dt}\langle p_x\rangle &= \frac{i}{\hbar}\langle[H,p_x]\rangle = \frac{i}{\hbar}\langle[V(x),p_x]\rangle \\
&= \frac{i}{\hbar}\langle i\hbar\frac{\partial V(x)}{\partial x}\rangle = -\langle\frac{\partial V(x)}{\partial x}\rangle
\end{aligned}$$

Similarly for y and z components. Therefore we have

$$\frac{\partial}{\partial t}\langle\vec{p}\rangle = -\langle\nabla V\rangle$$

2.22.24 Solution of Coupled Linear ODEs

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

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

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

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

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

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

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

or

$$\begin{aligned}
x_1 &= \frac{1}{2}(x_2 + x_3) \\
\frac{1}{2}(x_2 + 3x_3) &= 2x_2 \\
3x_3 &= 3x_2
\end{aligned}$$

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

$$A = \begin{pmatrix} -\frac{2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix}$$

Now the formal solution to the differential equation is

$$x(t) = e^{A(t)} x(0)$$

We then have

$$\begin{aligned}
e^{A(t)} &= \begin{pmatrix} -\frac{2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} e^{-t} & 0 & 0 \\ 0 & e^{-t} & 0 \\ 0 & 0 & e^{2t} \end{pmatrix} \begin{pmatrix} -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \\
&= \begin{pmatrix} \frac{2}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{\sqrt{3}}e^{2t} \\ -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & \frac{2}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{\sqrt{3}}e^{2t} \\ -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & \frac{2}{3}e^{-t} + \frac{1}{\sqrt{3}}e^{2t} \end{pmatrix}
\end{aligned}$$

and finally

$$x(t) = \begin{pmatrix} \frac{2}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{\sqrt{3}}e^{2t} \\ -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & \frac{2}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{\sqrt{3}}e^{2t} \\ -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & -\frac{1}{3}e^{-t} + \frac{1}{3}e^{2t} & \frac{2}{3}e^{-t} + \frac{1}{\sqrt{3}}e^{2t} \end{pmatrix} x(0)$$

(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 (λ_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

$$\begin{aligned} x(t) = e^{-t} &\left(-\frac{2}{\sqrt{6}} a + \frac{1}{\sqrt{6}} b + \frac{1}{\sqrt{6}} c \right) v_{-1,1} \\ + e^{-t} &\left(\frac{1}{\sqrt{2}} b - \frac{1}{\sqrt{2}} c \right) v_{-1,2} \\ + e^{2t} &\left(\frac{1}{\sqrt{3}} a + \frac{1}{\sqrt{3}} b + \frac{1}{\sqrt{3}} c \right) v_2 \end{aligned}$$

2.22.25 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:

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

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

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

This clearly has the solution

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

and also

$$-b + ic = 0 \quad , \quad -ib - c = 0 \rightarrow b = ic$$

Hence, if we choose $a = 0$ in this case we have for $\lambda = 1$

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

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

$$b + ic = 0 \quad , \quad -ib + c = 0 \rightarrow b = -ic$$

Then for $\lambda = -1$ we have

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

We then have the projection operators

$$P_{-1} = \frac{1}{2} \begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix} \begin{pmatrix} 0 & i & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & 1 \end{pmatrix}$$

$$P_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix} \begin{pmatrix} 0 & -i & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & i/2 \\ 0 & -i/2 & 1/2 \end{pmatrix}$$

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

$$P_1 P_{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & i/2 \\ 0 & -i/2 & 1/2 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1/2 & -i/2 \\ 0 & i/2 & 1/2 \end{pmatrix} = 0$$

2.22.26 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 σ_i of a matrix A there exist some unit normalized vector u_i such that

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

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

We have

$$P^\dagger P = P^2 = P$$

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

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

(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

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

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

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

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 R^2?

We compute

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

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 $N^\dagger N$ 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

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

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 3

Probability

3.6 Problems

3.6.1 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) $Prob$(dry)

(2) $Prob$(dry AND windy)

(3) $Prob$(wet OR windy)

(1) $P(dry) = P(\sim wet) = 1 - P(wet) = 1 - 0.3 = 0.7$

(2) $P(dry \wedge windy) = P(windy) - P(\sim dry \wedge windy)$
$= P(windy) - P(wet \wedge windy) = 0.4 - 0.2 = 0.2$

(3) $P(wet \vee windy = P(wet) + P(windy) - P(wet \wedge windy)$
$= 0.4 + 0.3 - 0.2 = 0.5$

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

We have

$$P(H \vee S) = P(H) + P(S) - P(H \wedge S) = 0.91 + 0.95 - 0.88 = 0.98$$

(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

$$P(RH\ larger) = \frac{15}{36}$$

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

$$P(A \wedge B) = P(A|B)P(B)$$

Thus,

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

(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 $P(A|B) = 2/3$.

(2) $P(B|A)$

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

(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 $P(A) = 1/2$. Two faces yield A and D (as it can be either way up) so $P(A \wedge D) = 1/3$. Finally,

$$P(D|A) = \frac{P(A \wedge D)}{P(A)} = \frac{2}{3}$$

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 $P(D|A) = 1/2$.

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 $P(A|B) = 2/7$. Here $A = A \wedge B$ and so

$$P(A) = P(A \wedge B) = P(A|B)P(B) = \frac{2}{7} \times \frac{3}{8} = \frac{3}{28}$$

(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

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

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

$$\begin{array}{ll} P(A|B \wedge C) = \frac{99}{100} \quad , & P(B|C) = \frac{95}{100} \\ P(\sim A|\sim B \wedge C) = \frac{30}{100} \quad , & P(\sim B|C) = \frac{5}{100} \end{array}$$

Therefore,

$$\begin{aligned} P(A|C) &= P(A|B \wedge C)P(B|C) + P(\sim A|\sim B \wedge C)P(\sim B|C) \\ &= \tfrac{99}{100}\tfrac{95}{100} + \tfrac{30}{100}\tfrac{5}{100} = \tfrac{9555}{10000} = 0.9555 \end{aligned}$$

(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. Hence

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

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

$$\begin{pmatrix} 4 \\ 4 \end{pmatrix} = 1$$

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.

3.6.2 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 $N_1S_2S_3$ means: 1^{st} card drawn is not a spade, 2^{nd} card drawn is a spade, 3^{rd} card drawn is a spade. In this notation, the possible ways of discarding 2 cards and *then* drawing a spade are:

$$S_1S_2S_3 \quad , \quad S_1N_2S_3 \quad , \quad N_1S_2S_3 \quad , \quad N_1N_2S_3$$

These events are mutually exclusive, therefore using

$$P(A \vee B) = P(A) + P(B)$$

i.e., we *add* their probabilities. Now to compute the probability of, say, $S_1N_2S_3$, we use the equation $P(A \wedge B) = P(A)P(B)$ 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

$$P(S_1N_2S_3) = \frac{13}{52} \times \frac{39}{51} \times \frac{12}{50}$$

Similarly,

$$\begin{aligned} P(S_1S_2S_3) &= \tfrac{13}{52} \times \tfrac{12}{51} \times \tfrac{11}{50} \\ P(N_1S_2S_3) &= \tfrac{39}{52} \times \tfrac{13}{51} \times \tfrac{12}{50} \\ P(N_1N_2S_3) &= \tfrac{39}{52} \times \tfrac{38}{51} \times \tfrac{13}{50} \end{aligned}$$

which gives

$$\begin{aligned} P(3^{rd}\ card\ is\ a\ spade) &= P(S_1N_2S_3) + P(S_1S_2S_3) + P(N_1S_2S_3) + P(N_1N_2S_3) \\ &= \tfrac{13}{52}\left[\tfrac{12(11+39)+39(12+38)}{51\times 50}\right] = \tfrac{1}{4} \end{aligned}$$

3.6.3 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

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

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

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 $= 364/365$. The probability that the 3^{rd} person has a different birthday from either of the first two is $= 363/365$, and so on. Now using the equation $P(A \wedge B) = P(A)P(B)$ the probability that the first two people have different birthdays and then that the third person has a still different birthday is the product

$$P(A \wedge B) = \frac{364}{365} \times \frac{363}{365} = \left(1 - \frac{1}{365}\right)\left(1 - \frac{2}{365}\right)$$

Continuing in this way for n people, we have

$$p = P(all\ different\ birthdays) = \left(1 - \frac{1}{365}\right)\left(1 - \frac{2}{365}\right)....\left(1 - \frac{n-1}{365}\right)$$

Now

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

and

$$ln\,(1-x) \approx -x \quad for \quad x << 1$$

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

$$ln(p) = -\frac{1}{365} - \frac{2}{365} - ... - \frac{n-1}{365} = -\frac{1+2+...+(n-1)}{365} = -\frac{n(n-1)}{2 \times 365}$$

If $p < 1/2$ or $ln(p) < ln(1/2) = -ln(2)$, 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 1/2 that two people will have the same birthday. For 50 people, the probability of coincidence is about 0.97

3.6.4 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!

3.6.5 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

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

If we define

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

then

$$P(n_H|M^n) = binomial(n_H, n, 0.5) - binomial(n_H + 1, n, 0.5)$$

and

$$P(m \leq n_H \leq s|M^n) = binomial(m, n, 0.5) - binomial(s + 1, n, 0.5)$$

Exactly 1/2 heads:

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

which clearly approaches zero as it should.

In range:

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

so that

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

but

$$P(\textit{to be in vicinity of } 1/2) \to 1 \;\; as \;\; N \to \infty$$

3.6.6 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 $P(A|B)P(B)$ = probability of selecting the right pocket and then selecting a nickel from it. Thus,

$$P(B) = P(right\ pocket) = \tfrac{1}{2} \text{ (two equally likely pockets)}$$
$$P(A|B) = P(nickel|right\ pocket) = \tfrac{3}{7} \text{ (3 nickels out of 7 coins)}$$
$$P(A|B)P(B) = \tfrac{1}{2} \times \tfrac{3}{7} = \tfrac{3}{14}$$

Now

$$\begin{aligned} P(A) = P(nickel) &= P(nickel|right)P(right) + P(nickel|left)P(left) \\ &= P(A|B)P(B) + P(A|\sim B)P(\sim B) \\ &= \tfrac{3}{7} \times \tfrac{1}{2} + \tfrac{2}{3} \times \tfrac{1}{2} = \tfrac{23}{42} \end{aligned}$$

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

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

3.6.7 Psychological Tests

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

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

and the *data*:

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

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

Let B = event that taxicab was actually blue. From Bayes' theorem, the correct answer is

$$\begin{aligned} P(B|D \wedge I) &= \tfrac{P(D|B \wedge I)P(B)}{P(D)} = \tfrac{(0.2)\times(0.85)}{P(D|B \wedge I)P(B) + P(D|\sim B \wedge I)P(\sim B)} \\ &= \tfrac{(0.2)\times(0.85)}{(0.2)\times(0.85)+(0.8)\times(0.15)} = \tfrac{17}{29} = 0.59 \end{aligned}$$

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 ($G \to B$ or $B \to G$), 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 $P(B|D \wedge I)$ 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.

3.6.8 Bayes Rules, Gaussians and Learning

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

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

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

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

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

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

where

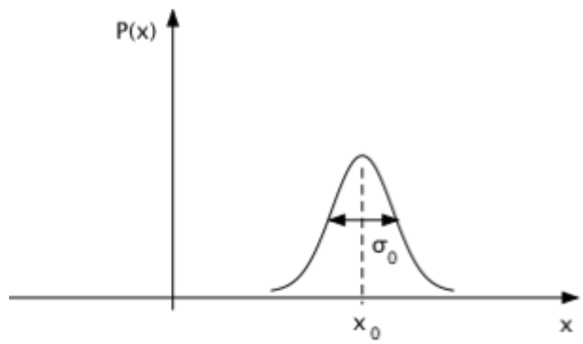
$$x' = x_0 + K_1(y - x_0) \ , \ \sigma'^2 = K_2\sigma_0^2 \ , \ K_1 = \frac{\sigma_0^2}{\sigma_0^2 + \Delta^2} \ , \ K_2 = \frac{\Delta^2}{\sigma_0^2 + \Delta^2}$$

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

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 Δx 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

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

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:

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

where

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

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

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

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

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

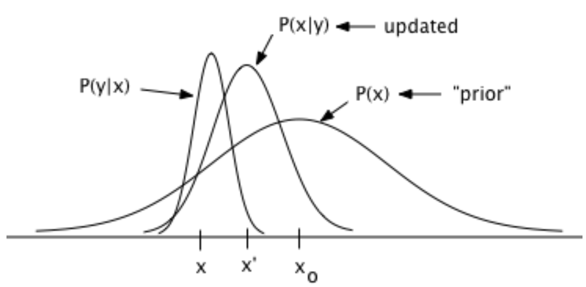
where $N(y, x_0)$ contains all the rest of the factors. Instead of keeping track of all of these factors we can just replace it by the correct normalization

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

where

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

Graphically we have



After the measurement, the new distribution is a *narrower* Gaussian *peaked closer to the actual position.* That is called *Bayes' learning.*

3.6.9 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 3.1:

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

Table 3.1: Berger's Burgers Details

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

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

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

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

$$1 = \sum_i P(A_i) \tag{3.1}$$

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

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

$$S = \sum_i P(A_i) \log_2 \left(\frac{1}{P(A_i)} \right) \tag{3.2}$$

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

$$\begin{aligned} 1 &= P(B) + P(C) + P(F) \\ 1.75 &= 1.00P(B) + 2.00P(C) + 3.00P(F) \end{aligned}$$

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

$$a \leq P(B) \leq b$$
$$c \leq P(C) \leq d$$
$$e \leq P(F) \leq f$$

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

$$P(C) = 0.75 - 2P(F)$$
$$P(B) = 0.25 + P(F)$$

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

$$0 < P(F) < 0.375 \text{ (expected value constraint)}$$

$$0 < P(C) < 0.75 \text{ (last equations)}$$

$$0.25 < P(B) < 0.625 \text{ (last equations)}$$

or

$$0.0 \leq P(F) \leq 0.375$$
$$0.0 \leq P(C) \leq 0.75$$
$$0.25 \leq P(B) \leq 0.625$$

(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

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

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.

$$\begin{aligned} \text{Average Calorie Count} &= 1000P(B) + 600P(C) + 400P(F) \\ &= 466.0 + 190.8 + 86.4 = 743.2 \end{aligned}$$

$$\begin{aligned} \text{Average Meals Cold} &= 0.5P(B) + 0.2P(C) + 0.1P(F) \\ &= 0.233 + 0.064 + 0.022 = 0.319 \end{aligned}$$

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.

3.6.10 Extended Menu at Berger's Burgers

Suppose now that Berger's extends its menu to include a Tofu option as shown in Table 3.2 below:

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

Table 3.2: 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

$$\begin{aligned}1 &= P(B) + P(C) + P(F) + P(T) \\ 2.50 &= 1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(T)\end{aligned}$$

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 α and β and then the Lagrangian function L:

$$\begin{aligned}L = S &- (\alpha - \log_2 e)(P(B) + P(C) + P(F) + P(T) - 1) \\ &- \beta(1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(T) - 2.50)\end{aligned}$$

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 α and β 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

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

so that

$$\begin{aligned}P(B) &= 2^{-\alpha}2^{-\beta} \\ P(C) &= 2^{-\alpha}2^{-2\beta} \\ P(F) &= 2^{-\alpha}2^{-3\beta} \\ P(T) &= 2^{-\alpha}2^{-8\beta}\end{aligned}$$

We can find α and β using

$$\begin{aligned}&P(B) + P(C) + P(F) + P(T) = 1 \\ &2^{-\alpha}(2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta}) = 1 \\ &\log_2\left(2^{-\alpha}(2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta})\right) = 0 \\ &\alpha = \log_2\left(2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta}\right)\end{aligned}$$

and

$$2^{\alpha}(1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(T)) = 2.50 \times 2^{\alpha}$$
$$1 \times 2^{-\beta} + 2 \times 2^{-2\beta} + 3 \times 2^{-3\beta} + 8 \times 2^{-8\beta} = 2.50 \times 2^{\alpha}$$
$$1 \times 2^{-\beta} + 2 \times 2^{-2\beta} + 3 \times 2^{-3\beta} + 8 \times 2^{-8\beta} = 2.50 \times (2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta})$$
$$1.50 \times 2^{-\beta} + 0.50 \times 2^{-2\beta} - 0.50 \times 2^{-8\beta} - 5.50 \times 2^{-8\beta} = 0$$

Finding the zeroes of the last equation gives us β and the value of β gives us α, which then determine the probabilities and the entropy. The computed values are

$$\beta = 0.2586\ bits/dollar$$
$$\alpha = 1.2371\ bits$$
$$P(B) = 0.3546$$
$$P(C) = 0.2964$$
$$P(F) = 0.2478$$
$$P(T) = 0.1011$$
$$S = 1.8835\ bits$$

3.6.11 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 Δt such that no more than one particle arrives in that interval. The probability for a particle to be in the interval Δt 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

$$\begin{aligned} P(n, t+\Delta t) &= P(n,t)P(0,\Delta t) + P(n-1,t)P(1,\Delta t) \\ &= P(n,t)(1 - R\Delta t) + P(n-1,t)(R\Delta t) \end{aligned}$$

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

$$P(n,t) = \frac{1}{n!}(Rt)^n e^{-Rt}$$

Histograms:

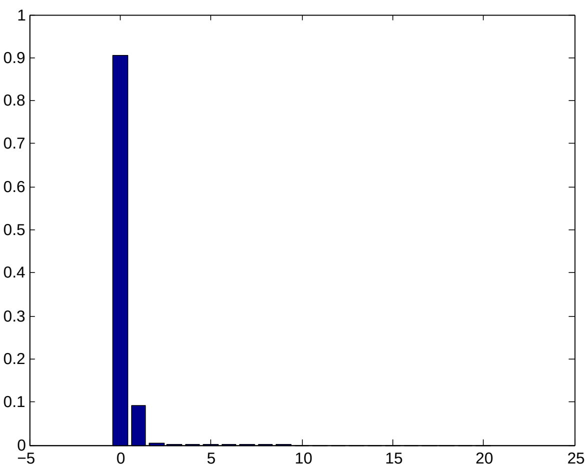


Figure 3.1: $Rt = 0.1$

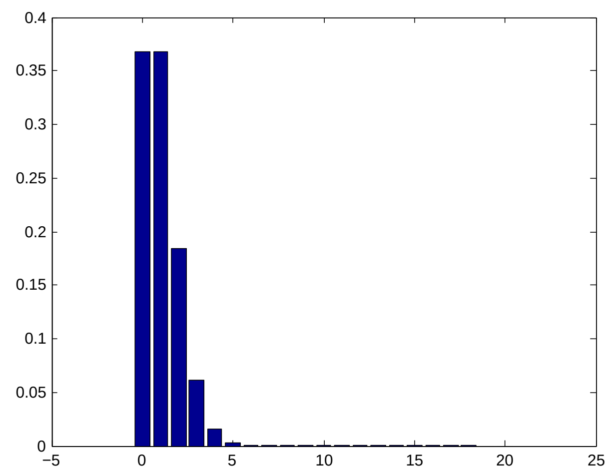


Figure 3.2: $Rt = 1.0$

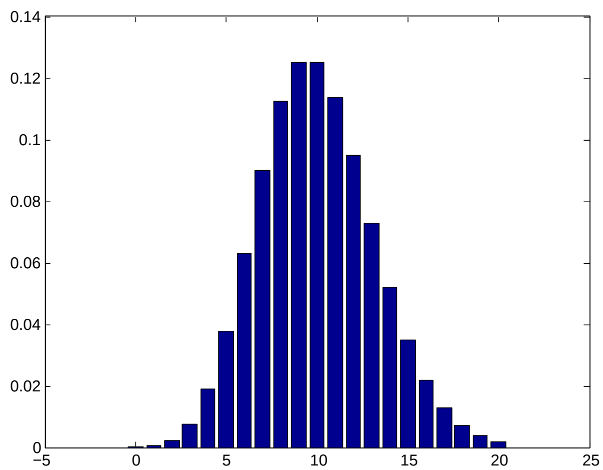


Figure 3.3: $Rt = 10.0$

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:

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

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

The expected value is

$$\begin{aligned}
\langle n \rangle &= \sum_{n=0}^{\infty} nP(n,t) = \sum_{n=0}^{\infty} \frac{n}{n!}(Rt)^n e^{-Rt} \\
&= \left(\sum_{n=0}^{\infty} \frac{1}{(n-1)!}(Rt)^n \right) e^{-Rt} = \left(\sum_{m=0}^{\infty} \frac{1}{m!}(Rt)^{m+1} \right) e^{-Rt} \\
&= Rt \left(\sum_{m=0}^{\infty} \frac{1}{m!}(Rt)^m \right) e^{-Rt} = Rt(e^{Rt})e^{-Rt} = Rt
\end{aligned}$$

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,

$$\begin{aligned}
\sigma_n^2 &= \langle n(n-1) \rangle + \langle n \rangle - \langle n \rangle^2 \\
&= (Rt)^2_R t - (Rt)^2 = Rt \to \sigma_n = \sqrt{Rt} = \sqrt{\langle n \rangle}
\end{aligned}$$

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 Δt: $p = R\Delta t = Rt/N$ which implies that

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

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

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

and

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

to get

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

which is the Poisson distribution.

3.6.12 Modeling Dice: Observables and Expectation Values

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

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

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

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

Thus, the expectation values of a and b are

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

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

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

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

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

and

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

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

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

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

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,

(1,1)	-	-	-	(5,5)	-
(2,1)(1,2)	(2,4)(4,2)	-	(4,5)(5,4)	-	-
(3,1)(1,3)	(3,3)	(3,5)(5,3)	-	-	-
(4,1)(2,2)(1,4)	(2,5)(5,2)	(4,4)	-	-	-
(1,5)(5,1)	-	-	-	-	-
(1,6)(2,3)(3,2)(6,1)	(2,6)(3,4)(4,3)(6,2)	(3,6)(6,3)	(4,6)(6,4)	(5,6)(6,5)	(6,6)

and thus,

$$\begin{aligned}\langle p\rangle &= \frac{1}{36}[1+2(2)+3(2)+4(3)+5(2)+6(4)+8(2)+9+10(2)+12(4)+15(2)+16+18(2)\\ &\qquad +20(2)+24(2)+25+30(2)+36]\\ &= \frac{1}{36}[1+4+6+12+10+24+16+9+20+48+30+16+36+40+48+25++60+36]\\ &= \frac{441}{36} = 12.25\end{aligned}$$

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).

3.6.13 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 $[0, 1/6, 1/6, 1/6, 1/6, 1/6]$. Via Bayes' rule,

$$\begin{aligned}Pr(a = i|s = 8) &= \frac{Pr(s = 8|a = i)Pr(a = i)}{Pr(s = 8)} = \frac{Pr(s = 8|a = i)\frac{1}{6}}{\frac{5}{36}}\\ &= Pr(s = 8|a = i)\frac{6}{5}\end{aligned}$$

The forward conditional probabilities are then

$$\begin{aligned}
Pr(s = 8|a = 1) &= 0 \\
Pr(s = 8|a = 2) = Pr(b = 6) &= \frac{1}{6} \\
Pr(s = 8|a = 3) = Pr(b = 5) &= \frac{1}{6} \\
Pr(s = 8|a = 4) = Pr(b = 4) &= \frac{1}{6} \\
Pr(s = 8|a = 5) = Pr(b = 3) &= \frac{1}{6} \\
Pr(s = 8|a = 6) = Pr(b = 2) &= \frac{1}{6}
\end{aligned}$$

(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 $15/2$.

3.6.14 Matrix Observables for Classical Probability

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

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

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

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

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

We have

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

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

(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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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,

$$v_1 v_2 = \begin{pmatrix} c_1 & 0 \\ 0 & d_1 \end{pmatrix} \begin{pmatrix} c_2 & 0 \\ 0 & d_2 \end{pmatrix} == \begin{pmatrix} c_1 c_2 & 0 \\ 0 & d_1 d_2 \end{pmatrix}$$

which is still in V, and clearly $v_1 v_2 = v_2 v_1$. 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 4

The Formulation of Quantum Mechanics

4.19 Problems

4.19.1 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 $\{|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_D\rangle\}$ and the real numbers $\{w_1, w_2, ..., w_D\}$.

Now, since the collection of states $\{|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_D\rangle\}$ is orthonormal, we have

$$\hat{P}_{|\psi_c\rangle}\hat{P}_{|\psi_d\rangle} = \delta_{cd}\hat{P}_{|\psi_d\rangle}$$

which implies that

$$\hat{\rho}^2 = \sum_{c=1}^{D}\sum_{d=1}^{D} w_c w_d \hat{P}_{|\psi_c\rangle}\hat{P}_{|\psi_d\rangle} = \sum_{c=1}^{D}\sum_{d=1}^{D} w_c w_d \delta_{cd}\hat{P}_{|\psi_d\rangle} = \sum_{d=1}^{D} w_d^2 \hat{P}_{|\psi_d\rangle}$$

But we assumed that $\hat{\rho}^2 = \hat{\rho}$ so that we must also have

$$\hat{\rho}^2 = \sum_{d=1}^{D} w_d \hat{P}_{|\psi_d\rangle}$$

or

$$\sum_{d=1}^{D} w_d^2 \hat{P}_{|\psi_d\rangle} = \sum_{d=1}^{D} w_d \hat{P}_{|\psi_d\rangle}$$

Now, multiply both sides by $\hat{P}_{|\psi_c\rangle}$ and use $\hat{P}_{|\psi_c\rangle}\hat{P}_{|\psi_d\rangle} = \delta_{cd}\hat{P}_{|\psi_d\rangle}$

$$\begin{aligned}
&\sum_{d=1}^{D} w_d^2 \hat{P}_{|\psi_c\rangle}\hat{P}_{|\psi_d\rangle} = \sum_{d=1}^{D} w_d \hat{P}_{|\psi_c\rangle}\hat{P}_{|\psi_d\rangle} \\
&\sum_{d=1}^{D} w_d^2 \delta_{cd} \hat{P}_{|\psi_d\rangle} = \sum_{d=1}^{D} w_d \delta_{cd} \hat{P}_{|\psi_d\rangle} \\
&(w_c^2 - w_c)\hat{P}_{|\psi_c\rangle} = 0 \quad \text{for all } c = 1, 2, ..., D
\end{aligned}$$

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, $\hat{\rho} = \hat{P}_{|\psi\rangle} = |\psi\rangle\langle\psi|$ for some vector $|\psi\rangle$ or $\hat{\rho}$ represents a state vector.

4.19.2 Pure and Nonpure States

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

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

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

for arbitrary θ.

(b) The nonpure state

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

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

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

$$\rho_\theta = \frac{1}{2}\begin{pmatrix} 1 & e^{i\theta} \\ e^{-i\theta} & 1 \end{pmatrix} \quad , \quad \rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Now look at the operator

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

We have

$$\rho_\theta\sigma_x = \frac{1}{2}\begin{pmatrix} e^{i\theta} & 1 \\ 1 & e^{-i\theta} \end{pmatrix} \quad , \quad \rho\sigma_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Therefore,

$$\langle\sigma_x\rangle_\theta = Tr\hat{\rho}_\theta\hat{\sigma}_x = \tfrac{1}{2}(e^{i\theta} + e^{-i\theta}) = \cos\theta \rightarrow \text{ represents a pure state}$$
$$\langle\sigma_x\rangle = Tr\hat{\rho}\hat{\sigma}_x = 0 \rightarrow \text{ represents a mixed state}$$

Therefore, for $\hat{\rho}$, $\left\langle \hat{B} \right\rangle = 0$ 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 $|\theta = 0\rangle = |\sigma_x = +1\rangle \rightarrow$ an eigenvector!

4.19.3 Probabilities

Suppose the operator

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

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

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

In problem 2.22.14 we showed that the eigenvalues of M are $\lambda = 0, \pm\sqrt{2}$ and the corresponding eigenvectors of M are

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

Now $\hat{P}_0 = |0\rangle \langle 0|$ and we have, in general,

$$\begin{aligned} Prob(M = 0|\rho) &= Tr(\hat{P}_0 \hat{\rho}) \\ &= \langle M = 0| \hat{P}_0 \hat{\rho} |M = 0\rangle + \left\langle M = \sqrt{2}\right| \hat{P}_0 \hat{\rho} \left|M = \sqrt{2}\right\rangle + \left\langle M = -\sqrt{2}\right| \hat{P}_0 \hat{\rho} \left|M = -\sqrt{2}\right\rangle \\ &= \langle M = 0| \hat{\rho} |M = 0\rangle \end{aligned}$$

(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

$$Prob(M = 0|\rho) = \langle M = 0| \hat{\rho} |M = 0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}^+ \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{3}{8}$$

(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

$$Prob(M = 0|\rho) = \langle M = 0| \hat{\rho} |M = 0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}^+ \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = 0$$

(c) We have

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

so that

$$Prob(M=0|\rho) = \langle M=0|\,\hat{\rho}\,|M=0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}^{+} \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} \end{bmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{2}$$

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

$$|1/2\rangle = |1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \,,\, |1/4\rangle = |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \,,\, |1/4\rangle = |-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Therefore the spectral decomposition of $\hat{\rho}$ is

$$\hat{\rho} = \frac{1}{2}|1\rangle\langle 1| + \frac{1}{4}|0\rangle\langle 0| + \frac{1}{4}|-1\rangle\langle -1| = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \frac{1}{4}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \frac{1}{4}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Now, using the $M-$basis, we have

$$\begin{aligned} |0\rangle &= \tfrac{1}{\sqrt{2}}\left(\left|M=\sqrt{2}\right\rangle - \left|M=-\sqrt{2}\right\rangle\right) \\ |\pm 1\rangle &= \tfrac{1}{2}\left(\left|M=\sqrt{2}\right\rangle + \left|M=-\sqrt{2}\right\rangle\right) \pm \tfrac{1}{\sqrt{2}}|M=0\rangle \end{aligned}$$

Therefore,

$$\begin{aligned} \hat{\rho} &= \frac{1}{2}|1\rangle\langle 1| + \frac{1}{4}|0\rangle\langle 0| + \frac{1}{4}|-1\rangle\langle -1| \\ &= \frac{1}{2}\left[\begin{array}{l} \frac{1}{4}\left|M=\sqrt{2}\right\rangle\left\langle M=\sqrt{2}\right| + \frac{1}{4}\left|M=-\sqrt{2}\right\rangle\left\langle M=-\sqrt{2}\right| + \frac{1}{2}|M=0\rangle\langle M=0| \\ +\frac{1}{4}\left|M=\sqrt{2}\right\rangle\left\langle M=-\sqrt{2}\right| + \frac{1}{4}\left|M=-\sqrt{2}\right\rangle\left\langle M=\sqrt{2}\right| + \frac{1}{2\sqrt{2}}\left|M=\sqrt{2}\right\rangle\langle M=0| \\ +\frac{1}{2\sqrt{2}}|M=0\rangle\left\langle M=\sqrt{2}\right| + \frac{1}{2\sqrt{2}}\left|M=-\sqrt{2}\right\rangle\langle M=0| + \frac{1}{2\sqrt{2}}|M=0\rangle\left\langle M=-\sqrt{2}\right| \end{array}\right] \\ &+ \frac{1}{4}\left[\begin{array}{l} \frac{1}{2}\left|M=\sqrt{2}\right\rangle\left\langle M=\sqrt{2}\right| + \frac{1}{2}\left|M=-\sqrt{2}\right\rangle\left\langle M=-\sqrt{2}\right| - \frac{1}{2}\left|M=\sqrt{2}\right\rangle\left\langle M=-\sqrt{2}\right| \\ -\frac{1}{2}\left|M=-\sqrt{2}\right\rangle\left\langle M=\sqrt{2}\right| \end{array}\right] \\ &+ \frac{1}{4}\left[\begin{array}{l} \frac{1}{4}\left|M=\sqrt{2}\right\rangle\left\langle M=\sqrt{2}\right| + \frac{1}{4}\left|M=-\sqrt{2}\right\rangle\left\langle M=-\sqrt{2}\right| + \frac{1}{2}|M=0\rangle\langle M=0| \\ +\frac{1}{4}\left|M=\sqrt{2}\right\rangle\left\langle M=-\sqrt{2}\right| + \frac{1}{4}\left|M=-\sqrt{2}\right\rangle\left\langle M=\sqrt{2}\right| - \frac{1}{2\sqrt{2}}\left|M=\sqrt{2}\right\rangle\langle M=0| \\ -\frac{1}{2\sqrt{2}}|M=0\rangle\left\langle M=\sqrt{2}\right| - \frac{1}{2\sqrt{2}}\left|M=-\sqrt{2}\right\rangle\langle M=0| - \frac{1}{2\sqrt{2}}|M=0\rangle\left\langle M=-\sqrt{2}\right| \end{array}\right] \end{aligned}$$

and we have

$$Prob(M=0|\rho) = \langle M=0|\,\hat{\rho}\,|M=0\rangle = \frac{1}{2}\frac{1}{2} + \frac{1}{4}\frac{1}{2} = \frac{3}{8}$$

as before.

4.19.4 Acceptable Density Operators

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

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

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

$$\rho_5 = \frac{1}{3}\,|u\rangle\langle u| + \frac{2}{3}\,|v\rangle\langle v| + \frac{\sqrt{2}}{3}\,|u\rangle\langle v| + \frac{\sqrt{2}}{3}\,|v\rangle\langle u|$$

$$\langle u \mid u\rangle = \langle v \mid v\rangle = 1 \text{ and } \langle u \mid v\rangle = 0$$

$$\rho_1 = \begin{bmatrix} \frac{1}{4} & \frac{3}{4} \\ \frac{3}{4} & \frac{3}{4} \end{bmatrix} \to \rho_1^2 = \begin{bmatrix} \frac{5}{8} & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{25} \end{bmatrix} \to Tr\rho_1^2 = \frac{7}{4} > 1 \to \text{ not acceptable}$$

$$\rho_2 = \begin{bmatrix} \frac{9}{25} & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{25} \end{bmatrix} \to \rho_2^2 = \rho_2 \to Tr\rho_2^2 = Tr\rho_2 = 1 \to \text{ pure state}$$

$$\rho_3 = \begin{bmatrix} \frac{9}{25} & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{25} \end{bmatrix} = |\psi_3\rangle\langle\psi_3| \to |\psi_3\rangle = \frac{1}{5}\begin{pmatrix} 3 \\ 4 \end{pmatrix}$$

$$\rho_4 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & \frac{1}{2} & 0 \\ \frac{1}{4} & 0 & 0 \end{bmatrix} \to \rho_4^2 \neq \rho_4 \to Tr\rho_4^2 = \frac{5}{8} < 1 \to \text{ a mixed state}$$

The eigenvalues of ρ_4 are $1/2, (1 \pm \sqrt{2})/4$ and the eigenvectors are

$$|1/2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad \left|\frac{1+\sqrt{2}}{4}\right\rangle = \begin{pmatrix} 0.92 \\ 0 \\ 0.38 \end{pmatrix} \quad , \quad \left|\frac{1-\sqrt{2}}{4}\right\rangle = \begin{pmatrix} -0.38 \\ 0 \\ 0.92 \end{pmatrix}$$

Spectral decomposition implies that

$$\hat{\rho}_4 = \frac{1}{2}\,|1/2\rangle\langle 1/2| + \frac{1+\sqrt{2}}{4}\left|\frac{1+\sqrt{2}}{4}\right\rangle\left\langle\frac{1+\sqrt{2}}{4}\right| + \frac{1-\sqrt{2}}{4}\left|\frac{1-\sqrt{2}}{4}\right\rangle\left\langle\frac{1-\sqrt{2}}{4}\right|$$

which corresponds to a mixed state.

$$\rho_5 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} \end{bmatrix} \to \rho_5^2 \neq \rho_5 \to Tr\rho_5^2 = \frac{1}{2} < 1 \to \text{ mixed state}$$

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

$$\begin{aligned}
&\rho_5^2 = \rho_5 \to Tr\rho_5^2 = Tr\rho_5 = 1 \to \text{ pure state} \\
&\rho_5 = \tfrac{1}{3}|u\rangle\langle u| + \tfrac{2}{3}|v\rangle\langle v| + \tfrac{\sqrt{2}}{3}|u\rangle\langle v| + \tfrac{\sqrt{2}}{3}|v\rangle\langle u| = |\psi_5\rangle\langle\psi_5| \\
&|\psi_5\rangle = \tfrac{1}{\sqrt{3}}|u\rangle + \sqrt{\tfrac{2}{3}}|v\rangle
\end{aligned}$$

4.19.5 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

$$\langle\psi|\hat{\rho}_1|\psi\rangle \geq 0 \quad , \quad \langle\psi|\hat{\rho}_2|\psi\rangle \geq 0$$

and we also have $0 \leq (1-r) \leq 1$. Therefore,

$$\langle\psi|\hat{\rho}|\psi\rangle = r\langle\psi|\hat{\rho}_1|\psi\rangle + (1-r)\langle\psi|\hat{\rho}_2|\psi\rangle$$

This is the sum of two numbers both of which are greater than or equal to zero. Therefore,

$$\langle\psi|\hat{\rho}|\psi\rangle \geq 0$$

The trace is a linear operation, so

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

Therefore, $\hat{\rho} = r\hat{\rho}_1 + (1-r)\hat{\rho}_2$ is a density matrix for all real numbers r such that $0 \leq r \leq 1$.

4.19.6 Unitary Operators

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

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

We have

$$\begin{aligned}
&\left\langle\tilde{\varphi} \mid \tilde{\psi}\right\rangle = \langle\varphi|U^+U|\psi\rangle = \langle\varphi \mid \psi\rangle = \langle\varphi|I|\psi\rangle \\
&\Rightarrow U^+U = I \\
&U^+\left|\tilde{\psi}\right\rangle = U^+U|\psi\rangle = I|\psi\rangle = |\psi\rangle \\
&\Rightarrow \langle\varphi \mid \psi\rangle = \langle\tilde{\varphi}|UU^+\left|\tilde{\psi}\right\rangle = \left\langle\tilde{\varphi} \mid \tilde{\psi}\right\rangle \\
&\Rightarrow UU^+ = I
\end{aligned}$$

(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

$$\begin{aligned}
&U = \exp(iA) \quad , \quad A\ Hermitian \\
&U = \sum_{n=0}^{\infty} \frac{1}{n!}(iA)^n \Rightarrow U^+ = \sum_{n=0}^{\infty} \frac{1}{n!}(-iA^+)^n = \sum_{n=0}^{\infty} \frac{1}{n!}(-iA)^n \\
&U^+ = \exp(-iA)
\end{aligned}$$

Thus,

$$\begin{aligned}
&U^+U = \exp(iA)\exp(-iA) = \exp(0) = I \\
&\Rightarrow U\ is\ unitary
\end{aligned}$$

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 = the Hamiltonian. Given a state at $t = 0$, $|\psi(0)\rangle$, let $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, which implies that

$$\begin{aligned}
&\frac{\partial}{\partial t}|\psi(t)\rangle = \frac{\partial U(t)}{\partial t}|\psi(0)\rangle \\
&\frac{\partial U(t)}{\partial t} = \frac{\partial e^{-iHt/\hbar}}{\partial t} = -\frac{iH}{\hbar}e^{-iHt/\hbar} = -\frac{iH}{\hbar}U(t) \\
&\frac{\partial}{\partial t}|\psi(t)\rangle = -\frac{iH}{\hbar}U(t)|\psi(0)\rangle = -\frac{iH}{\hbar}|\psi(t)\rangle \\
&i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle
\end{aligned}$$

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 $\||\psi(0)\rangle\|^2 = \langle\psi(0) \mid \psi(0)\rangle = 1$, i.e., normalized to a total probability of all possible alternatives. At later times, this total probability must be conserved. This implies that

$$\begin{aligned}
&\||\psi(t)\rangle\|^2 = \langle\psi(t) \mid \psi(t)\rangle = 1 \\
&\langle\psi(t) \mid \psi(t)\rangle = \langle\psi(0) \mid \psi(0)\rangle
\end{aligned}$$

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 $\hat{U}(t) = \sum_n e^{-iE_nt/\hbar}|u_n\rangle\langle u_n|$. 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,

$$U(t) = U\hat{I} = U\sum_n |u_n\rangle \langle u_n| = \sum_n e^{-iHt/\hbar} |u_n\rangle \langle u_n|$$
$$U(t) = \sum_n e^{-iE_n t/\hbar} |u_n\rangle \langle u_n| = \sum_n e^{-i\omega_n t} |u_n\rangle \langle u_n|$$

and

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = \left(\sum_n e^{-i\omega_n t} |u_n\rangle \langle u_n|\right)|\psi(0)\rangle = \sum_n e^{-i\omega_n t} |u_n\rangle \langle u_n \mid \psi(0)\rangle$$

so that

$$c_n = \langle u_n \mid \psi(0)\rangle$$

4.19.7 More Density Matrices

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

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

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

Clearly ρ is hermitian and $Tr\rho = 1$. This is almost sufficient for ρ 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 ρ is diagonal. Such a transformation preserves the trace. In this diagonal basis, ρ 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 ρ 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 ρ 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

$$\begin{aligned}
\langle\psi|\rho|\psi\rangle &= (\alpha^*\langle 1| + \beta^*\langle 2| + \gamma^*\langle 3|)(a|1\rangle\langle 1| + b|2\rangle\langle 2| + c|3\rangle\langle 3|)(\alpha|1\rangle + \beta|2\rangle + \gamma|3\rangle) \\
&= (\alpha^*, \beta^*, \gamma^*)\frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \\
&= 2|\alpha|^2 + |\beta|^2 + |\gamma|^2 + 2\mathrm{Re}(\alpha^*\beta) + 2\mathrm{Re}(\alpha^*\gamma)
\end{aligned}$$

which can never be negative by virtue of the relation

$$|x|^2 + |y|^2 + 2\mathrm{Re}(x^*y) = |x+y|^2 \geq 0$$

Therefore, ρ is a valid density operator.

To determine whether ρ is a pure or mixed state, we consider

$$Tr(\rho^2) = \frac{1}{16}Tr\begin{pmatrix} 6 & 3 & 3 \\ 3 & 2 & 1 \\ 3 & 1 & 2 \end{pmatrix} = \frac{5}{8}$$

This is not equal to one, so ρ is a mixed state.

(b) Given the ensemble described by ρ, 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

$$\langle J_z\rangle = Tr(\rho J_z) = \frac{1}{4}Tr\begin{pmatrix} 2 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix} = \frac{3}{4}$$

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

We need

$$\langle J_z^2\rangle = Tr(\rho J_z^2) = \frac{1}{4}Tr\begin{pmatrix} 2 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \frac{3}{4}$$

and then

$$\Delta J_z = \sqrt{\langle J_z^2\rangle - \langle J_z\rangle^2} = \sqrt{11/16} = 0.829$$

4.19.8 Scale Transformation

Space is invariant under the scale transformation

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

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

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

where $\hat{D}$ is the *dilation* generator. Determine the commutators $\left[\hat{D}, \hat{x}\right]$ and $\left[\hat{D}, \hat{p}_x\right]$ between the generators of dilation and space displacements. Determine the operator $\hat{D}$. Not all the laws of physics are invariant under dilation, so the symmetry is less common than displacements or rotations. You will need to use the identity in Problem 4.19.11.

Under a scale transformation we have

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

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

$$\hat{x}U^{-1}\,|x'\rangle = xU^{-1}\,|x'\rangle = U^{-1}x\,|x'\rangle \to \hat{U}\hat{x}U^{-1}\,|x'\rangle = x\,|x'\rangle$$

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

$$\hat{U}\hat{x}U^{-1} = e^{-c}\hat{x} \to e^c\hat{x} = U^{-1}\hat{x}\hat{U} = e^{ic\hat{D}}\hat{x}e^{-ic\hat{D}}$$

Now using the identity in Problem 6.19.11 we have

$$e^{ic\hat{D}}\hat{x}e^{-ic\hat{D}} = \hat{x} + c\left[i\hat{D}, \hat{x}\right] + \frac{1}{2}c^2\left[i\hat{D}, \left[i\hat{D}, \hat{x}\right]\right] + ...$$

and also

$$e^{c}\hat{x} = \hat{x}\left(1 + c + \frac{1}{2}c^{2} + + + + +\right)$$

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 $\left[\hat{x}, \hat{D}\right] = i\hat{x}$ we get

$$\left[\left[\hat{D}, \hat{p}_x\right], \hat{x}\right] = \hbar$$

which says that

$$\left[\hat{D}, \hat{p}_x\right] = i\hat{p}_x$$

This says that

$$\hat{D} = \frac{1}{2\hbar}\left(\hat{x}\hat{p}_x + \hat{p}_x\hat{x}\right)$$

since

$$\left[i\hat{D}, \hat{x}\right] = \tfrac{i}{2\hbar}\left[\hat{x}\hat{p}_x + \hat{p}_x\hat{x}, \hat{x}\right] = \tfrac{i}{2\hbar}\left(\left[\hat{x}\hat{p}_x, \hat{x}\right] + \left[\hat{p}_x\hat{x}, \hat{x}\right]\right) = \tfrac{i}{2\hbar}\left(-i\hbar\hat{x} - i\hbar\hat{x}\right) = \hat{x}$$
$$\left[-i\hat{D}, \hat{p}_x\right] = \tfrac{-i}{2\hbar}\left[\hat{x}\hat{p}_x + \hat{p}_x\hat{x}, \hat{p}_x\right] = \tfrac{-i}{2\hbar}\left(\left[\hat{x}\hat{p}_x, \hat{p}_x\right] + \left[\hat{p}_x\hat{x}, \hat{p}_x\right]\right) = \tfrac{-i}{2\hbar}\left(i\hbar\hat{p}_x + i\hbar\hat{p}_x\right) = \hat{p}_x$$

and $\hat{D}$ must be hermitian.

4.19.9 Operator Properties

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

We have

$$U = e^{iH}$$

Then

$$\hat{U}^{+} = e^{-i\hat{H}^{+}} = e^{-i\hat{H}}$$
$$\hat{U}^{+}\hat{U} = e^{-i\hat{H}}e^{i\hat{H}} = \hat{I}$$

so that $\hat{U}$ is unitary.

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

There exists a unitary matrix U that diagonalizes H, i.e.,

$$U^{+}HU = D$$

Then

$$U^+H^2U = U^+HUU^+HU = D^2$$

and

$$U^+H^nU = U^+HU.......U^+HU = D^n$$

We then have

$$U^+e^{iH}U = \sum_{n=0}^{\infty} U^+(iH)^nU = \sum_{n=0}^{\infty} U^+(iD)^nU = U^+e^{iD}U$$

Now since D is diagonal and since the product of diagonal matrices is also diagonal we get

$$\left(e^{iD}\right)_{ii} = \sum_{n=0}^{\infty} \frac{(iD)_{ii}^n}{n!} = e^{iD_{ii}} \rightarrow e^{iD} = \begin{bmatrix} e^{i\lambda_1} & 0 & 0 & 0 & ... & 0 \\ 0 & e^{i\lambda_2} & 0 & 0 & ... & 0 \\ 0 & 0 & e^{i\lambda_3} & 0 & ... & 0 \\ 0 & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & ... \\ 0 & 0 & 0 & ... & ... & e^{i\lambda_n} \end{bmatrix}$$

and

$$\begin{aligned} \det(U) &= \det(e^{iH}) = \det(e^{iH}UU^+) = \det(U^+e^{iH}U) = \det(e^{iD}) \\ &= e^{i\lambda_1}e^{i\lambda_2}e^{i\lambda_3}......e^{i\lambda_n} = e^{i(\lambda_1+\lambda_2+\lambda_3+...+\lambda_n)} = e^{iTrD} \end{aligned}$$

Now

$$Tr(U^+HU) = Tr(HUU^+) = TrH = TrD = \sum_i \lambda_i$$

so that

$$\det(U) = e^{iTrD} = e^{iTrH}$$

4.19.10 An Instantaneous Boost

The unitary operator

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

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:

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

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

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

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

The *restricted* Galilean transformation is given by the unitary operator $\hat{U}(\vec{v}) = e^{i\vec{v}\cdot\hat{\vec{G}}}$ such that

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

This restricted transformation is *instantaneous* and thus causes no change in the position!

The full Galilean transformation is given by $\hat{U}(\vec{v},t) = e^{i\vec{v}\cdot\hat{\vec{G}}_t}$ such that

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

Method 1:

$$\hat{U}\hat{\vec{Q}}\hat{U}^{-1} = e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{\vec{Q}}e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{\vec{Q}} - \vec{v}t\hat{I}$$

In general, however,

$$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{\vec{Q}}e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{\vec{Q}} + i\left[\vec{v}\cdot\hat{\vec{G}}_t, \hat{\vec{Q}}\right] + ...$$

which implies that

$$\hat{\vec{G}}_t = -\frac{\hat{\vec{P}}}{\hbar}t + \frac{1}{\hbar}\hat{\vec{Q}}$$

that is,

$$\begin{aligned} i\left[\vec{v}\cdot\hat{\vec{G}}_t, \hat{\vec{Q}}\right] &= iv_x\left[\hat{G}_{tx}, \hat{x}\right] + iv_y\left[\hat{G}_{ty}, \hat{y}\right] + iv_z\left[\hat{G}_{tz}, \hat{z}\right] \\ &= iv_x\left(-\frac{t}{\hbar}\right)\left[\hat{P}_x, \hat{x}\right] + iv_y\left[\hat{P}_y, \hat{y}\right] + iv_z\left[\hat{P}_z, \hat{z}\right] = -\vec{v}t\hat{I} \end{aligned}$$

as expected.

Method 2: The desired transformation $\hat{U}(\vec{v},t) = e^{i\vec{v}\cdot\hat{\vec{G}}_t}$ 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

$$\hat{\vec{G}}_t = M\hat{\vec{Q}} - t\hat{\vec{P}} = \text{ (instantaneous boost) + (space translation)}$$

We let $\hbar = 1$ for convenience. We have

$$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{Q}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{Q}_\alpha + \left[i\vec{v}\cdot\hat{\vec{G}}_t, \hat{Q}_\alpha\right] + (\text{ higher order terms})$$

The commutator has the value

$$\left[i\vec{v}\cdot\hat{\vec{G}}_t, \hat{Q}_\alpha\right] = -i\left[i\vec{v}\cdot\hat{\vec{P}}t, \hat{Q}_\alpha\right] = -v_\alpha t\hat{I}$$

Since this is a multiple of the identity operator, all the higher order terms vanish above and we get

$$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{Q}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{Q}_\alpha - v_\alpha t\hat{I}$$

Similarly,

$$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{P}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{P}_\alpha + \left[i\vec{v}\cdot\hat{\vec{G}}_t, \hat{P}_\alpha\right] + (\text{ higher order terms})$$
$$\left[i\vec{v}\cdot\hat{\vec{G}}_t, \hat{P}_\alpha\right] = -i\left[iM\vec{v}\cdot\hat{\vec{Q}}, \hat{P}_\alpha\right] = -Mv_\alpha\hat{I}$$

Again all higher order terms are zero and we have

$$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{P}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{P}_\alpha - Mv_\alpha t\hat{I}$$

Dividing the equation by M gives the correct transformation equation for the velocity operator $\hat{V}_\alpha = \hat{P}_\alpha/M$. So the assumption

$$\hat{\vec{G}}_t = M\hat{\vec{Q}} - t\hat{\vec{P}}$$

is correct.

Commutators: Consider $\hat{G}_{t1}$ with $\hat{H}$. We have

$$e^{i\varepsilon\hat{H}}e^{i\varepsilon\hat{G}_{t1}}e^{-i\varepsilon\hat{H}}e^{-i\hat{G}_{t1}} = \hat{I} + \varepsilon^2\left[\hat{G}_{t1}, \hat{H}\right]$$

This is unchanged from result in text with $\hat{G}_1$ and so this commutator does not change and similarly for all others.

4.19.11 A Very Useful Identity

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

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

There is a clever way(see Problem 6.19.12 below if you are having difficulty) to do this problem using ODEs and not just brute-force multiplying everything out. Straightforward expansion/regrouping

$$\begin{aligned}
\hat{f}(x) = e^{x\hat{A}}\hat{B}e^{-x\hat{A}} &= \left(\sum_n \frac{(x\hat{A})^n}{n!}\right)\hat{B}\left(\sum_n \frac{(-x\hat{A})^n}{n!}\right) \\
&= \left(1 + x\hat{A} + \frac{1}{2}x^2\hat{A}^2 + ...\right)\hat{B}\left(1 - x\hat{A} + \frac{1}{2}x^2\hat{A}^2 - ....\right) \\
&= \hat{B} + x\left[\hat{A}, \hat{B}\right] + x^2\left(-\hat{A}\hat{B}\hat{A} + \frac{1}{2}(\hat{A}^2\hat{B} - \hat{B}\hat{A}^2)\right) + ... \\
&= \hat{B} + x\left[\hat{A}, \hat{B}\right] + \frac{1}{2}x^2\left(\hat{A}(\hat{A}\hat{B} - \hat{B}\hat{A}) - (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{A}\right) + ... \\
&= \hat{B} + x\left[\hat{A}, \hat{B}\right] + \frac{1}{2}x^2\left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] + ...
\end{aligned}$$

4.19.12 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

$$e^A B e^{-A} = \sum_0^\infty \frac{1}{n!} \underbrace{[A, [A, ...[A,}_{n} B \underbrace{]....]]}_{n}$$
$$= B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + ...$$

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

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

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

(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

$$B(1) = B + \int_0^1 \frac{d}{dt} B(t) dt$$
$$B(1) = B + \int_0^1 [A, B(t)] dt$$
$$\sum_{n=0}^\infty B_n = B_0 + \sum_{n=0}^\infty [A, B_n] \int_0^1 t^n \, dt$$
$$\sum_{n=0}^\infty B_n = B_0 + \sum_{n=0}^\infty [A, B_n] \frac{1}{n+1}$$
$$\sum_{n=1}^\infty B_n = \sum_{n=0}^\infty [A, B_n] \frac{1}{n+1}$$
$$\sum_{n=1}^\infty B_n = \sum_{n=1}^\infty [A, B_{n-1}] \frac{1}{n}$$
$$\to B_n = \frac{1}{n}[A, B_{n-1}]$$

(c) Show by induction that

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

We have

$$\begin{aligned}B_n &= \frac{1}{n}[A,B_{n-1}] = \frac{1}{n}\left[A,\frac{1}{n-1}[A,B_{n-2}]\right] \\ &= \frac{1}{n(n-1)}[A,[A,B_{n-2}]] = ... = \frac{1}{n(n-1)....(n-n+1)}[A,.......[A,B_{n-n}]] \\ &= \frac{1}{n!}[A,[A,.....[A,B]....]] \quad \text{(with n nested commutators)}\end{aligned}$$

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

$$\begin{aligned}e^A B e^{-A} &= B(1) = \sum_{n=0}^{\infty} B_n \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}[A,[A,.....[A,B]....]]\end{aligned}$$

(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

$$\begin{aligned}e^{ipa/\hbar}xe^{-ipa/\hbar} &= \sum_{n=0}^{\infty}\frac{1}{n!}[A,[A,.....[A,x]....]] \\ &= \sum_{n=0}^{\infty}\frac{a^n}{n!}\left(\frac{i}{\hbar}\right)^n [p,[p,.....[p,x]....]]\end{aligned}$$

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

$$\hat{f}(x) = \hat{f}(0) + x\left.\frac{d\hat{f}(x)}{dx}\right|_{x=0} + \frac{1}{2}x^2\left.\frac{d^2\hat{f}(x)}{dx^2}\right|_{x=0} + ...$$

In this case, we can write

$$\frac{d\hat{f}(x)}{dx} = \hat{A}e^{x\hat{A}}\hat{B}e^{-x\hat{A}} - e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\hat{A} = \left[\hat{A},\hat{f}(x)\right]$$

This implies that

$$\frac{d^2\hat{f}(x)}{dx^2} = \frac{d}{dx}\left[\frac{df}{dx}\right] = \frac{d}{dx}\left[\hat{A},\hat{f}(x)\right] = \left[\hat{A},\frac{df}{dx}\right] = \left[\hat{A},\left[\hat{A},\hat{f}(x)\right]\right]$$

and so on. Since $\hat{f}(0) = \hat{B}$ we get

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

We note that this is the solution of the first-order operator differential equation

$$\frac{d\hat{f}(x)}{dx} = \left[\hat{A},\hat{f}(x)\right]$$

with boundary condition $\hat{f}(0) = \hat{B}$.

4.19.13 Another Very Useful Identity

Prove that

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

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

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

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

We define $\hat{f}(x) = e^{x\hat{A}}e^{x\hat{B}}$. We then have

$$\begin{aligned}\frac{d\hat{f}(x)}{dx} &= \hat{A}e^{x\hat{A}}e^{x\hat{B}} + e^{x\hat{A}}\hat{B}e^{x\hat{B}} = \hat{A}e^{x\hat{A}}e^{x\hat{B}} + e^{x\hat{A}}\hat{B}e^{-x\hat{A}}e^{x\hat{A}}e^{x\hat{B}} \\ &= \left(\hat{A} + e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\right)e^{x\hat{A}}e^{x\hat{B}} = \left(\hat{A} + e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\right)\hat{f}(x)\end{aligned}$$

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

$$\frac{d\hat{f}(x)}{dx} = \left(\hat{A} + e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\right)\hat{f}(x) = \left(\hat{A} + \hat{B} + \left[\hat{A},\hat{B}\right]x\right)\hat{f}(x)$$

This equation has the solution

$$\hat{f}(x) = e^{x\hat{A}}e^{x\hat{B}} = e^{(\hat{A}+\hat{B})x + \frac{1}{2}x^2\left[\hat{A},\hat{B}\right]}$$

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

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

(behave like ordinary numbers in algebra). Therefore, we finally get

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

4.19.14 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 $Tr\hat{\rho}^2 = 1 \quad (not \quad < 1)$ 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

$$\frac{dTr\hat{\rho}^2}{dt} = -\frac{2i}{\hbar}Tr\left(\hat{\rho}\left[\hat{H},\hat{\rho}\right]\right) = \frac{2i}{\hbar}Tr\left(\hat{\rho}\hat{H}\hat{\rho} - \hat{H}\hat{\rho}\hat{\rho}\right) = 0$$

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,

$$\begin{aligned}
Tr\hat{\rho}^2(t) &= Tr(\hat{\rho}(t)\hat{\rho}(t)) = Tr\left(\hat{U}\hat{\rho}(t_0)\hat{U}^{-1}\hat{U}\hat{\rho}(t_0)\hat{U}^{-1}\right) \\
&= Tr\left(\hat{U}\hat{\rho}(t_0)\hat{I}\hat{\rho}(t_0)\hat{U}^{-1}\right) = Tr\left(\hat{U}\hat{\rho}(t_0)\hat{\rho}(t_0)\hat{U}^{-1}\right) \\
&= Tr\left(\hat{\rho}(t_0)\hat{I}\hat{\rho}(t_0)\hat{U}^{-1}\hat{U}\right) = Tr\left(\hat{\rho}(t_0)I\hat{\rho}(t_0)\right) = Tr\hat{\rho}^2(t_0)
\end{aligned}$$

4.19.15 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

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

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

$$S(f, \hat{p}^+g) = S(\hat{p}f, g) = \int_{-\infty}^{\infty} dx\, [-if^*(x)]'g(x) = i \int_{-\infty}^{\infty} dx\, f'^*(x)g(x)$$

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 $\left[\hat{M}, \hat{q}\right] = 0$, it follows that $\left[\hat{M}, \hat{q}^n\right] = 0$, $n = 1, 2, 3, ...$ and hence that

$$\left[\hat{M}, e^{it\hat{q}}\right] = 0$$

Thus, any function of the operator $\hat{q}$ that has a Fourier transform,

$$f(\hat{q}) = \int_{-\infty}^{\infty} dt\, \tilde{f}(t) e^{it\hat{q}}$$

also commutes with $\hat{M}$. For such a function,

$$\hat{M} f(\hat{q}) g(x) = f(\hat{q}) \hat{M} g(x)$$

Since $\hat{q} g(x) = x g(x)$, $\hat{q}^n g(x) = x^n g(x)$ 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

$$\begin{aligned}
&\hat{p}\hat{M} g(x) = \hat{M}\hat{p} g(x) = -i\hat{M} g'(x) = -i g'(x) m(x) \\
&\hat{p}\hat{M} g(x) = \hat{p} g(x) m(x) = -i\tfrac{d}{dx}(g(x) m(x)) \\
&-i\tfrac{d}{dx}(g(x) m(x)) = -i g'(x) m(x) \\
&\tfrac{d}{dx}(g(x) m(x)) = g'(x) m(x)
\end{aligned}$$

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.

4.19.16 More About the Density Operator

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

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

the density matrix ρ is hermitian, hence diagonal in some basis. Work in such a basis. In this basis, ρ 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 ρ.

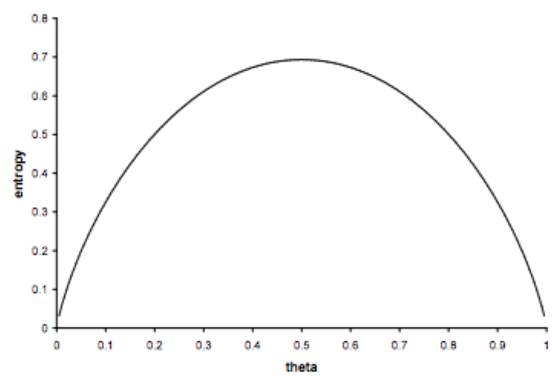


Figure 4.1: The entropy as a function of θ

The entropy for a pure state, with $\theta = 1$ or $\theta = 0$, is zero. The entropy increases as the state becomes *less pure*, reacing 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 ρ a mixture of two ensembles ρ_1 and ρ_2:

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

As an example, suppose

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

in some basis. Prove that

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

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

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 mat 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:

$$\rho = \theta\rho_1 + (1-\theta)\rho_2 = \frac{1}{2}\begin{pmatrix} 1 & 1-\theta \\ 1-\theta 1 & \end{pmatrix}$$

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:

$$\begin{aligned} s(\rho) - [\theta s(\rho_1) + (1-\theta)s(\rho_2)] &= -\left(1-\frac{\theta}{2}\right)\ln\left(1-\frac{\theta}{2}\right) - \left(-\frac{\theta}{2}\right)\ln\left(-\frac{\theta}{2}\right) - \theta\ln 2 \\ &= \ln\left[\left(1-\frac{\theta}{2}\right)^{1-\theta/2}\left(\frac{\theta}{2}\right)^{\theta/2} 2^{\theta}\right] \end{aligned}$$

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 θ equal to 0:

$$\begin{aligned}
0 &= \frac{d}{d\theta}\left(1-\frac{\theta}{2}\right)^{1-\theta/2}(2\theta)^{\theta/2} \\
&= \frac{d}{d\theta}exp\left[\left(1-\frac{\theta}{2}\right)\ln\left(1-\frac{\theta}{2}\right)+\left(\frac{\theta}{2}\right)\ln(2\theta)\right] \\
&= -\frac{1}{2}\ln(1-\theta/2)+\frac{1}{2}\ln(2\theta)-\frac{1}{2}+\frac{2}{4} \\
&= \ln(2\theta)-\ln(1-\theta/2)
\end{aligned}$$

Thus, the maximum occurs at $\theta = 2/5$. At this value of θ, $s)\rho) = 0.500$, and $\theta s(\rho_1) + (1-\theta)s(\rho_2) = (2/5)\ln 2 = 0.277$. The theorem holds.

4.19.17 Entanglement and the Purity of a Reduced Density Operator

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

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

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

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

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

$$\begin{aligned}
\rho &= |\Psi_{AB}\rangle\langle\Psi_{AB}| \\
&= \cos^2\theta\,|\Psi_{00}\rangle\langle\Psi_{00}| + \cos\theta\sin\theta\,|\Psi_{00}\rangle\langle\Psi_{11}| + \cos\theta\sin\theta\,|\Psi_{11}\rangle\langle\Psi_{00}| + \sin^2\theta\,|\Psi_{11}\rangle\langle\Psi_{11}|
\end{aligned}$$

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,

$$\begin{aligned}\tilde{\rho}_A &= Tr_B\rho = \langle 0_B|\,\rho\,|0_B\rangle + \langle 1_B|\,\rho\,|1_B\rangle \\ &= \cos^2\theta\,|0_A\rangle\langle 0_A| + \sin^2\theta\,|1_A\rangle\langle 1_A|\end{aligned}$$

and then

$$\tilde{\rho}_A^2 = \cos^4\theta\,|0_A\rangle\langle 0_A| + \sin^4\theta\,|1_A\rangle\langle 1_A|$$

so that

$$\zeta = Tr[\tilde{\rho}_A^2] = \cos^4\theta + \sin^4\theta$$

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

$$\cos^3\theta\sin\theta = \sin^3\theta\cos\theta \to \cos^2\theta = \sin^2\theta$$

For $0 \le \theta \le \pi/2$, this equation is satisfied for $\theta = \pi/4$, $\cos^2\theta = \sin^2\theta = 1/2$ and also $\zeta = 1/2$. At $\theta = \pi/4$,

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

which we recognize as a highly entangled state. Since for $\theta = 0$ we have

$$|\Psi_{AB}\rangle \to |0_A\rangle \otimes |0_B\rangle$$

which is unentangled and $\zeta \to 1$, we see clearly that entangled states are associated with smaller purity for the reduced density operator.

4.19.18 The Controlled-Not Operator

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

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

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

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

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

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

We start by writing out

$$
\begin{aligned}
U_{AB} &= P_0^A \otimes I^B + P_1^A \otimes \sigma_x^B \\
&= |0_A\rangle \langle 0_A| \otimes |0_B\rangle \langle 0_B| + |0_A\rangle \langle 0_A| \otimes |1_B\rangle \langle 1_B| \\
&\quad + |1_A\rangle \langle 1_A| \otimes |0_B\rangle \langle 1_B| + |1_A\rangle \langle 1_A| \otimes |1_B\rangle \langle 0_B| \\
&= |0_A\rangle \otimes |0_B\rangle \langle 0_A| \otimes \langle 0_B| + |0_A\rangle \otimes |1_B\rangle \langle 0_A| \otimes \langle 1_B| \\
&\quad + |1_A\rangle \otimes |0_B\rangle \langle 1_A| \otimes \langle 1_B| + |1_A\rangle \otimes |1_B\rangle \langle 1_A| \otimes \langle 0_B|
\end{aligned}
$$

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

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

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.

4.19.19 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

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

such that the *output* state

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

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

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

A general factorizable input state has the form

$$\begin{aligned}\left|\Psi_{AB}^{in}\right\rangle &= (a_0 |0_A\rangle + a_1 |1_A\rangle) \otimes (b_0 |0_B\rangle + b_1 |1_B\rangle) \\ &= a_0 b_0 |0_A\rangle \otimes |0_B\rangle + a_0 b_1 |0_A\rangle \otimes |1_B\rangle + a_1 b_0 |1_A\rangle \otimes |0_B\rangle + a_1 b_1 |1_A\rangle \otimes |1_B\rangle\end{aligned}$$

where $|a_0|^2 + |a_1|^2 = |b_0|^2 + |b_1|^2 = 1$. if we apply U_{AB} to this state we get

$$\begin{aligned}\left|\Psi_{AB}^{out}\right\rangle &= U_{AB} \left|\Psi_{AB}^{in}\right\rangle \\ &= a_0 b_0 |0_A\rangle \otimes |0_B\rangle + a_0 b_1 |0_A\rangle \otimes |1_B\rangle + a_1 b_0 |1_A\rangle \otimes |1_B\rangle + a_1 b_1 |1_A\rangle \otimes |0_B\rangle\end{aligned}$$

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

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

while in the latter we get

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

In either case it is straightforward to verify that $Tr[\tilde{\rho}_A^2] = 1/2$.

4.19.20 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 $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$,

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

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

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

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

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

so

$$
\begin{aligned}
|0_a 1_b\rangle &= \left(\cos\frac{\phi}{2}\left|\tilde{0}_a\right\rangle - \sin\frac{\phi}{2}\left|\tilde{1}_a\right\rangle\right) \otimes \left(\sin\frac{\phi}{2}\left|\tilde{0}_a\right\rangle + \cos\frac{\phi}{2}\left|\tilde{1}_a\right\rangle\right) \\
&= \sin\frac{\phi}{2}\cos\frac{\phi}{2}\left|\tilde{0}_a\tilde{0}_b\right\rangle + \cos^2\frac{\phi}{2}\left|\tilde{0}_a\tilde{1}_b\right\rangle \\
&\quad - \sin^2\frac{\phi}{2}\left|\tilde{1}_a\tilde{0}_b\right\rangle - \sin\frac{\phi}{2}\cos\frac{\phi}{2}\left|\tilde{1}_a\tilde{1}_b\right\rangle
\end{aligned}
$$

$$
\begin{aligned}
|1_a 0_b\rangle &= \left(\sin\frac{\phi}{2}\left|\tilde{0}_a\right\rangle + \cos\frac{\phi}{2}\left|\tilde{1}_a\right\rangle\right) \otimes \left(\cos\frac{\phi}{2}\left|\tilde{0}_a\right\rangle - \sin\frac{\phi}{2}\left|\tilde{1}_a\right\rangle\right) \\
&= \sin\frac{\phi}{2}\cos\frac{\phi}{2}\left|\tilde{0}_a\tilde{0}_b\right\rangle - \sin^2\frac{\phi}{2}\left|\tilde{0}_a\tilde{1}_b\right\rangle \\
&\quad + \cos^2\frac{\phi}{2}\left|\tilde{1}_a\tilde{0}_b\right\rangle - \sin\frac{\phi}{2}\cos\frac{\phi}{2}\left|\tilde{1}_a\tilde{1}_b\right\rangle
\end{aligned}
$$

and

$$
|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_a 1_b\rangle - |1_a 0_b\rangle) = \frac{1}{\sqrt{2}}(\left|\tilde{0}_a\tilde{1}_b\right\rangle - \left|\tilde{1}_a\tilde{0}_b\right\rangle)
$$

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 $|0_a 1_b\rangle$ go from

$$
\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}
$$

to

$$
\begin{pmatrix} \sin\frac{\phi}{2}\cos\frac{\phi}{2} \\ \cos^2\frac{\phi}{2} \\ -\sin^2\frac{\phi}{2} \\ -\sin\frac{\phi}{2}\cos\frac{\phi}{2} \end{pmatrix}
$$

4.19.21 Matrix Representations

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

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

For parts (a) -(c), let

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

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

Expanding this out in the joint-state basis,

$$\begin{aligned}
\rho_{AB} &= \frac{3}{8}\left|0_A\right\rangle\left\langle 0_A\right| \otimes \frac{1}{2}\left(\left|0_B\right\rangle + \left|1_B\right\rangle\right)\left(\left\langle 0_B\right| + \left\langle 1_B\right|\right) \\
&\quad + \frac{5}{8}\left|1_A\right\rangle\left\langle 1_A\right| \otimes \frac{1}{2}\left(\left\langle 0_B\right| - \left\langle 1_B\right|\right)\left(\left|0_B\right\rangle - \left|1_B\right\rangle\right) \\
&= \frac{3}{8}\left|0_A\right\rangle\left\langle 0_A\right| \otimes \frac{1}{2}(\left|0_B\right\rangle\left\langle 0_B\right| + \left|1_B\right\rangle\left\langle 0_B\right| + \left|0_B\right\rangle\left\langle 1_B\right| + \left|1_B\right\rangle\left\langle 1_B\right|) \\
&\quad + \frac{5}{8}\left|1_A\right\rangle\left\langle 1_A\right| \otimes \frac{1}{2}(\left|0_B\right\rangle\left\langle 0_B\right| - \left|1_B\right\rangle\left\langle 0_B\right| - \left|0_B\right\rangle\left\langle 1_B\right| + \left|1_B\right\rangle\left\langle 1_B\right|) \\
&= \frac{3}{16}(\left|0_a 0_b\right\rangle\left\langle 0_a 0_b\right| + \left|0_a 1_b\right\rangle\left\langle 0_a 0_b\right| + \left|0_a 0_b\right\rangle\left\langle 0_a 1_b\right| + \left|0_a 1_b\right\rangle\left\langle 0_a 1_b\right|) \\
&\quad + \frac{5}{16}(\left|1_a 0_b\right\rangle\left\langle 1_a 1_b\right| - \left|1_a 0_b\right\rangle\left\langle 0_a 0_b\right| - \left|1_a 0_b\right\rangle\left\langle 1_a 1_b\right| + \left|1_a 1_b\right\rangle\left\langle 1_a 1_b\right|) \\
&\leftrightarrow \frac{1}{16}\begin{pmatrix} 3 & 3 & 0 & 0 \\ 3 & 3 & 0 & 0 \\ 0 & 0 & 5 & -5 \\ 0 & 0 & -5 & 5 \end{pmatrix}
\end{aligned}$$

Alternatively, we could have written

$$\rho_{ab} = \frac{3}{16}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{5}{16}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

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

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

We have

$$P_0^B \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad , \quad P_1^B \leftrightarrow \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

so

$$I^A \otimes P_0^B \leftrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad , \quad I^A \otimes P_1^B \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Hence

$$
\begin{aligned}
&\left(I^A \otimes P_0^B\right) \rho_{AB} \left(I^A \otimes P_0^B\right) \\
&\quad = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 3 & 3 & 0 & 0 \\ 3 & 3 & 0 & 0 \\ 0 & 0 & 5 & -5 \\ 0 & 0 & -5 & 5 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
&\quad = \frac{1}{16} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
&\left(I^A \otimes P_1^B\right) \rho_{AB} \left(I^A \otimes P_1^B\right) \\
&\quad = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 3 & 3 & 0 & 0 \\ 3 & 3 & 0 & 0 \\ 0 & 0 & 5 & -5 \\ 0 & 0 & -5 & 5 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
&\quad = \frac{1}{16} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5 \end{pmatrix}
\end{aligned}
$$

and their sum is

$$
\left(I^A \otimes P_0^B\right) \rho_{AB} \left(I^A \otimes P_0^B\right) + \left(I^A \otimes P_1^B\right) \rho_{AB} \left(I^A \otimes P_1^B\right) \leftrightarrow \frac{1}{16} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 5 \end{pmatrix}
$$

(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:

$$
\begin{aligned}
\rho_{AB} &= \frac{3}{16}(|0_a 0_b\rangle \langle 0_a 0_b| + |0_a 1_b\rangle \langle 0_a 0_b| + |0_a 0_b\rangle \langle 0_a 1_b| + |0_a 1_b\rangle \langle 0_a 1_b|) \\
&\quad + \frac{5}{16}(|1_a 0_b\rangle \langle 1_a 1_b| - |1_a 0_b\rangle \langle 0_a 0_b| - |1_a 0_b\rangle \langle 1_a 1_b| + |1_a 1_b\rangle \langle 1_a 1_b|) \\
\tilde{\rho}_A &= \frac{3}{16}(|0_a\rangle \langle 0_a| + |0_a\rangle \langle 0_a|) + \frac{5}{16}(|1_a\rangle \langle 1_a| + |1_a\rangle \langle 1_a|) \\
&= \frac{3}{8} |0_a\rangle \langle 0_a| + \frac{5}{8} |1_a\rangle \langle 1_a|
\end{aligned}
$$

Thus, in matrix representation

$$
\tilde{\rho}_A = \frac{1}{8} \begin{pmatrix} 3 & 0 \\ 0 & 5 \end{pmatrix}
$$

4.19.22 Practice with Dirac Language for Joint Systems

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

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

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

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

where

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

Express your answer in Dirac language.

We are looking for O^A such that

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

For the specific state we are given,

$$\begin{aligned}
\langle \Psi_{AB}| O^A \otimes I^B |\Psi_{AB}\rangle &= \frac{1}{2}(\langle 0_A 0_B| + \langle 1_A 1_B|) O^A \otimes I^B (|0_A 0_B\rangle + |1_A 1_B\rangle) \\
&= \frac{1}{2}\left(\langle 0_a| O^A |0_a\rangle + \langle 1_a| O^A |1_a\rangle\right)
\end{aligned}$$

$$\begin{aligned}
\langle \Psi_{AB}| O^A \otimes P_0^B |\Psi_{AB}\rangle &= \frac{1}{2}(\langle 0_A 0_B| + \langle 1_A 1_B|) O^A \otimes P_0^B (|0_A 0_B\rangle + |1_A 1_B\rangle) \\
&= \frac{1}{2}\langle 0_a| O^A |0_a\rangle
\end{aligned}$$

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

$$o_{00} |0_a\rangle \langle 0_a| + o_{01} |0_a\rangle \langle 1_a| + o_{10} |1_a\rangle \langle 0_a| + o_{11} |1_a\rangle \langle 1_a|$$

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

$$O^A = a |0_a\rangle \langle 0_a| + (b + ic) |0_a\rangle \langle 1_a| + (b - ic) |1_a\rangle \langle 0_a| \quad a, b, c \in R$$

(b) Consider the specific operator

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

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

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

The most general form of a joint state vector is

$$|\Psi'_{AB}\rangle = c_{00}\,|0_A 0_B\rangle + c_{01}\,|0_A 1_B\rangle + c_{10}\,|1_A 0_B\rangle + c_{11}\,|1_A 1_B\rangle$$

so

$$\begin{aligned} X^A \otimes I^B |\Psi'_{AB}\rangle &= c_{00}(|0_a\rangle\langle 1_a| + |1_a\rangle\langle 0_a|)\,|0_A 0_B\rangle + c_{01}(|0_a\rangle\langle 1_a| + |1_a\rangle\langle 0_a|)\,|0_A 1_B\rangle \\ &\quad + c_{10}(|0_a\rangle\langle 1_a| + |1_a\rangle\langle 0_a|)\,|1_A 0_B\rangle + c_{11}(|0_a\rangle\langle 1_a| + |1_a\rangle\langle 0_a|)\,|1_A 1_B\rangle \\ &= c_{00}\,|I_a\rangle \otimes |0_b\rangle + c_{01}\,|I_a\rangle \otimes |1_b\rangle + c_{10}\,|0_a\rangle \otimes |0_b\rangle + c_{11}\,|0_a\rangle \otimes |1_b\rangle \\ &= c_{10}\,|0_a 0_b\rangle + c_{11}\,|0_a 1_b\rangle + c_{00}\,|1_a 0_b\rangle + c_{01}\,|1_a 1_b\rangle \end{aligned}$$

and

$$\begin{aligned} \langle\Psi'_{AB}| X^A \otimes I^B |\Psi'_{AB}\rangle &= c_{00}^* c_{10} + c_{01}^* c_{11} + c_{10}^* c_{00} + c_{11}^* c_{01} \\ &= 2Re[c_{00}^* c_{10} + c_{01}^* c_{11}] \end{aligned}$$

With the projected form, however,

$$(I^A \otimes P_0^B)\,\langle\Psi'_{AB}| = c_{00}\,|0_a 0_b\rangle + c_{10}\,|1_a 0_b\rangle$$

and

$$\begin{aligned} X^A \otimes I^B (I^A \otimes P_0^B)\,|\Psi'_{AB}\rangle &= c_{00}(|0_a\rangle\langle 1_a| + |1_a\rangle\langle 0_a|)\,|0_a 0_b\rangle \\ &\quad + c_{10}(|0_a\rangle\langle 1_a| + |1_a\rangle\langle 0_a|)\,|1_a 0_b\rangle \\ &= (c_{00}\,|1_a\rangle + c_{10}\,|0_a\rangle)\,|0_b\rangle \end{aligned}$$

so

$$\begin{aligned} \langle\Psi'_{AB}| X^A \otimes I^B (I^A \otimes P_0^B)\,|\Psi'_{AB}\rangle &= c_{00}^* c_{10} + c_{10}^* c_{00} \\ &= 2Re[c_{00}^* c_{10}] \end{aligned}$$

Comparing the two results, we only need $Re[c_{00}^* c_{10}] \neq 0$.

(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

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

We have

$$|\Psi'_{AB}\rangle = c_{00}\,|0_A 0_B\rangle + c_{01}\,|0_A 1_B\rangle + c_{10}\,|1_A 0_B\rangle + c_{11}\,|1_A 1_B\rangle$$

$$\langle \Psi'_{AB}| = c_{00}^* \langle 0_A 0_B| + c_{01}^* \langle 0_A 1_B| + c_{10}^* \langle 1_A 0_B| + c_{11}^* \langle 1_A 1_B|$$

together with the constraint $Re[c_{00}^* c_{10}] \neq 0$. We compute

$$\begin{aligned}
|\Psi'_{AB}\rangle \langle \Psi'_{AB}| = c_{00} |0_A 0_B\rangle &(c_{00}^* \langle 0_A 0_B| + c_{01}^* \langle 0_A 1_B| + c_{10}^* \langle 1_A 0_B| + c_{11}^* \langle 1_A 1_B|) \\
+ c_{01} |0_A 1_B\rangle &(c_{00}^* \langle 0_A 0_B| + c_{01}^* \langle 0_A 1_B| + c_{10}^* \langle 1_A 0_B| + c_{11}^* \langle 1_A 1_B|) \\
+ c_{10} |1_A 0_B\rangle &(c_{00}^* \langle 0_A 0_B| + c_{01}^* \langle 0_A 1_B| + c_{10}^* \langle 1_A 0_B| + c_{11}^* \langle 1_A 1_B|) \\
+ c_{11} |1_A 1_B\rangle &(c_{00}^* \langle 0_A 0_B| + c_{01}^* \langle 0_A 1_B| + c_{10}^* \langle 1_A 0_B| + c_{11}^* \langle 1_A 1_B|)
\end{aligned}$$

and

$$\begin{aligned}
\tilde{\rho}_A &= Tr_B\left[|\Psi'_{AB}\rangle \langle \Psi'_{AB}|\right] \\
&= c_{00} |0_a\rangle (c_{00}^* \langle 0_a| + c_{10}^* \langle 1_a|) + c_{01} |0_a\rangle (c_{01}^* \langle 0_a| + c_{11}^* \langle 1_a|) \\
&\quad + c_{10} |1_a\rangle (c_{00}^* \langle 0_a| + c_{10}^* \langle 1_a|) + c_{11} |1_a\rangle (c_{01}^* \langle 0_a| + c_{11}^* \langle 1_a|) \\
&= (|c_{00}|^2 + |c_{01}|^2) |0_a\rangle \langle 0_a| + (c_{00} c_{10}^* + c_{01} c_{11}^*) |0_a\rangle \langle 1_a| \\
&\quad + (c_{10} c_{00}^* + c_{11} c_{01}^*) |1_a\rangle \langle 0_a| + (|c_{10}|^2 + |c_{11}|^2) |1_a\rangle \langle 1_a|
\end{aligned}$$

Since we require $Re[c_{00}^* c_{10}] \neq 0$, it follows that $|c_{11}|^2 > 0$. It then becomes clear that, for example, we cannot achieve

$$\tilde{\rho}_A |0_a\rangle \langle 0_a|$$

since this would require $|c_{00}|^2 + |c_{01}|^2 = 1$, but by normalization $|c_{00}|^2 + |c_{01}|^2 \leq 1 - |c_{11}|^2$

4.19.23 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

$$\frac{1}{\sqrt{2}}(|0_a 0_b\rangle + |1_a 1_b\rangle)$$

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

$$p \quad : \quad \left|\Psi_{AB}^{out}\right\rangle = \frac{1}{\sqrt{2}}(|0_a 0_b\rangle - |1_a 1_b\rangle)$$

$$1-p \quad : \quad \left|\Psi_{AB}^{out}\right\rangle = \frac{1}{\sqrt{2}}(|0_a 0_b\rangle + |1_a 1_b\rangle)$$

The corresponding density operator is

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

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

$$O = I^A \otimes (|0_B\rangle\langle 0_B| - |1_B\rangle\langle 1_B|)$$

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 (± 1) are equally likely. using the projection postulate we can associate

$$+1 \;:\; \left|\Psi_{AB}^0\right\rangle \frac{(I^A \otimes |0_b\rangle\langle 0_b|)\left|\Psi_{AB}^0\right\rangle}{\sqrt{\langle\Psi_{AB}^0|(I^A \otimes |0_b\rangle\langle 0_b|)|\Psi_{AB}^0\rangle}} = |0_A 0_B\rangle$$

$$-1 \;:\; \left|\Psi_{AB}^0\right\rangle \frac{(I^A \otimes |1_b\rangle\langle 1_b|)\left|\Psi_{AB}^0\right\rangle}{\sqrt{\langle\Psi_{AB}^0|(I^A \otimes |1_b\rangle\langle 1_b|)|\Psi_{AB}^0\rangle}} = |1_A 1_B\rangle$$

so we can simply set

$$\rho_{AB} = \frac{1}{2}|0_A 0_B\rangle\langle 0_A 0_B| + \frac{1}{2}|1_A 1_B\rangle\langle 1_A 1_B|$$

4.19.24 Complete Sets of Commuting Observables

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

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

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

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

constitutes a valid CSCO.

First we check which observables commute.

$$\begin{aligned}
[O_\alpha, O_\beta] &= O_\alpha O_\beta - O_\beta O_\alpha \\
&= \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0
\end{aligned}$$

Likewise,

$$\begin{aligned}
[O_\alpha, O_\gamma] &= O_\alpha O_\gamma - O_\gamma O_\alpha \\
&= \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \neq 0
\end{aligned}$$

Finally,

$$\begin{aligned}
[O_\beta, O_\gamma] &= O_\beta O_\gamma - O_\gamma O_\beta \\
&= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0
\end{aligned}$$

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.

$$O_\alpha \;:\; 0 = \det\begin{pmatrix} 1-\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix}$$

$$\rightarrow \lambda^2(1-\lambda) = \lambda(\lambda(1-\lambda)+1) = 0$$

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_β and O_γ 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_β and O_γ:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \;:\; (1,0)\;,\; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \;:\; (1,1)\;,\; \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \;:\; (0,1)$$

So, finally, the valid CSCO's are $\{O_\alpha\}$, $\{O_\alpha, O_\beta\}$, and $\{O_\beta, O_\gamma\}$.

4.19.25 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)

$$\begin{aligned}
[O_\alpha, H] &= \varepsilon_0[O_\alpha, O_\alpha + O_\beta] = 0 \\
[O_\beta, H] &= \varepsilon_0[O_\beta, O_\alpha + O_\beta] = 0 \\
[O_\gamma, H] &= \varepsilon_0[O_\gamma, O_\alpha + O_\beta] \qquad\qquad = \varepsilon_0[O_\gamma, O_\alpha] + \varepsilon_0[O_\gamma, O_\beta] \\
&= \varepsilon_0[O_\gamma, O_\alpha] \neq 0
\end{aligned}$$

Hence, only $\{O_\alpha\}$ and $\{O_\alpha, O_\beta\}$ are conserved.

Chapter 5

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

5.5 Problems

5.5.1 Change the Basis

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

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

We have

$$\begin{aligned} |R\rangle &= \tfrac{1}{\sqrt{2}}(|x\rangle + i\,|y\rangle) \quad , \quad |L\rangle = \tfrac{1}{\sqrt{2}}(|x\rangle - i\,|y\rangle) \\ |45^\circ\rangle &= \tfrac{1}{\sqrt{2}}(|x\rangle + |y\rangle) \quad , \quad |135^\circ\rangle = \tfrac{1}{\sqrt{2}}(-|x\rangle + |y\rangle) \end{aligned}$$

Therefore, inverting we have

$$\begin{aligned} |x\rangle &= \langle R \mid x\rangle |R\rangle + \langle L \mid x\rangle |L\rangle = \tfrac{1}{\sqrt{2}}(|R\rangle + |L\rangle) \\ |y\rangle &= \langle R \mid y\rangle |R\rangle + \langle L \mid y\rangle |L\rangle = \tfrac{i}{\sqrt{2}}(-|R\rangle + |L\rangle) \end{aligned}$$

and

$$\begin{aligned} |x\rangle &= \langle 45^\circ \mid x\rangle |45^\circ\rangle + \langle 135^\circ \mid x\rangle |135^\circ\rangle = \tfrac{1}{\sqrt{2}}(|45^\circ\rangle + |135^\circ\rangle) \\ |y\rangle &= \langle 45^\circ \mid y\rangle |45^\circ\rangle + \langle 135^\circ \mid y\rangle |135^\circ\rangle = \tfrac{1}{\sqrt{2}}(-|45^\circ\rangle + |135^\circ\rangle) \end{aligned}$$

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

We have

$$\hat{P}_{vert} = \hat{P}_y = |y\rangle \langle y|$$

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

$$\begin{aligned}\hat{P}_{vert} = \hat{P}_y = |y\rangle \langle y| &= \left(\frac{i}{\sqrt{2}}(-|R\rangle + |L\rangle)\right)\left(\frac{-i}{\sqrt{2}}(-\langle R| + \langle L|)\right) \\ &= \frac{1}{2}\left(|R\rangle \langle R| - |R\rangle \langle L| - |L\rangle \langle R| + |L\rangle \langle L|\right)\end{aligned}$$

5.5.2 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

$$\begin{aligned}|\theta\rangle &= \cos\theta\,|x\rangle + \sin\theta\,|y\rangle \\ |30\rangle &= \tfrac{\sqrt{3}}{2}\,|x\rangle + \tfrac{1}{2}\,|y\rangle \\ |45\rangle &= \tfrac{1}{\sqrt{2}}\,|x\rangle + \tfrac{1}{\sqrt{2}}\,|y\rangle \\ |60\rangle &= \tfrac{1}{2}\,|x\rangle + \tfrac{\sqrt{3}}{2}\,|y\rangle\end{aligned}$$

Then

$$\begin{aligned}P(x \to 45 \to y) &= |\langle y \mid y\rangle \langle y \mid 45\rangle \langle 45 \mid x\rangle|^2 \\ &= |\langle y \mid 45\rangle \langle 45 \mid x\rangle|^2 = \left|\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{4}\end{aligned}$$

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.

$$\begin{aligned}P(x \to 30 \to 60 \to y) &= |\langle y \mid y\rangle \langle y \mid 60\rangle \langle 60 \mid 30\rangle \langle 30 \mid x\rangle|^2 \\ &= |\langle y \mid 60\rangle \langle 60 \mid 30\rangle \langle 30 \mid x\rangle|^2 \\ &= \left|\frac{\sqrt{3}}{2}\frac{\sqrt{3}}{2}\frac{\sqrt{3}}{2}\right|^2 = \frac{27}{64}\end{aligned}$$

5.5.3 Calcite Crystal

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

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

We have

$$\begin{aligned}
&|in\rangle = \cos\theta\,|o\rangle + \sin\theta\,|e\rangle \\
&|out\rangle = \hat{T}\,|in\rangle = \left(e^{ik_o\ell}\,|o\rangle\,\langle o| + e^{ik_e\ell}\,|e\rangle\,\langle e|\right)|in\rangle \\
&|final\rangle = |L\rangle = \tfrac{1}{\sqrt{2}}(|o\rangle - i\,|e\rangle)
\end{aligned}$$

$$P = \text{ probability of emerging LCP (in } |L\rangle \text{ state) } = |\langle L \mid out\rangle|^2$$

$$P = \frac{1}{2}\left|e^{ik_o\ell}\cos\theta + ie^{ik_e\ell}\sin\theta\right|^2 = \frac{1}{2}\left(1 + \sin 2\theta\sin\left(k_o - k_e\right)\ell\right)$$

Now

$$\begin{aligned}
&\ell = 10^{-2}\,cm \quad , \quad \tfrac{c}{\omega} = 5000\,\overset{o}{A} = 5\times10^{-5}\,cm \\
&n_e = 1.50 \to k_e\ell = \tfrac{\omega}{c}n_e\ell = 300 \\
&n_o = 1.65 \to k_o\ell = \tfrac{\omega}{c}n_o\ell = 330 \\
&\sin\left(k_o - k_e\right)\ell = \sin 30 = -0.9880
\end{aligned}$$

so that

$$P = \frac{1}{2}\left(1 - 0.988\sin 2\theta\right)$$

5.5.4 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:

$$R(\theta)\left|\varphi\right\rangle = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix}$$
$$= \begin{pmatrix} \cos\theta\cos\varphi + \sin\theta\sin\varphi \\ -\sin\theta\cos\varphi + \cos\theta\sin\varphi \end{pmatrix} = \begin{pmatrix} \cos(\varphi-\theta) \\ \sin(\varphi-\theta) \end{pmatrix} = \left|\varphi-\theta\right\rangle$$

and

$$\theta = -\frac{\pi\ell}{36} \to 5^\circ \ per\ cm$$

Since

$$R^+R = I \to R^+ = R^{-1} \to R \text{ is unitary}$$

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 $\left|RCP\right\rangle$ and $\left|LCP\right\rangle$ with eigenvalues $e^{i\theta}$ and $e^{-i\theta}$.

Proof:

$$\det\begin{pmatrix} \cos\theta-\lambda & \sin\theta \\ -\sin\theta & \cos\theta-\lambda \end{pmatrix} = 0 = (\cos\theta-\lambda)^2 + \sin^2\theta$$
$$0 = \cos^2\theta + \sin^2\theta - 2\lambda\cos\theta + \lambda^2 = \lambda^2 - 2\lambda\cos\theta + 1$$
$$\lambda = \tfrac{2\cos\theta\pm\sqrt{4\cos^2\theta-4}}{2} = \cos\theta \pm i\sin\theta = e^{\pm i\theta}$$

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = e^{\pm i\theta}\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = (\cos\theta \pm i\sin\theta)\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix}$$
$$a_\pm\cos\theta + b_\pm\sin\theta = a_\pm\cos\theta \pm ia_\pm\sin\theta$$
$$b_\pm = \pm ia_\pm$$
$$\left|e^{\pm i\theta}\right\rangle = a_\pm\begin{pmatrix} 1 \\ \pm i \end{pmatrix} = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm i \end{pmatrix}$$
$$\left|e^{i\theta}\right\rangle = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} = \left|R\right\rangle \quad , \quad \left|e^{-i\theta}\right\rangle = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \left|L\right\rangle$$

In general, we can write

$$\left|in\right\rangle = \left|R\right\rangle\left\langle R \mid in\right\rangle + \left|L\right\rangle\left\langle L \mid in\right\rangle$$

so that

$$\left|out\right\rangle = R(\theta)\left|in\right\rangle = R(\theta)\left|R\right\rangle\left\langle R \mid in\right\rangle + R(\theta)\left|L\right\rangle\left\langle L \mid in\right\rangle$$
$$= e^{i\theta}\left|R\right\rangle\left\langle R \mid in\right\rangle + e^{-i\theta}\left|L\right\rangle\left\langle L \mid in\right\rangle = e^{-i\frac{\pi\ell}{36}}\left|R\right\rangle\left\langle R \mid in\right\rangle + e^{-i\frac{\pi\ell}{36}}\left|L\right\rangle\left\langle L \mid in\right\rangle$$

5.5.5 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

$$|in\rangle = R(\theta)\,|x\rangle = \cos\theta\,|x\rangle + \sin\theta\,|y\rangle \quad , \quad \theta = 30^\circ$$

$$\begin{array}{l} P_{Ry} = \left|\langle y \mid R\rangle \langle R \mid in\rangle\right|^2 = \text{probabilityof } |out\rangle = |y\rangle \text{ via } |R\rangle \\ P_{Ly} = \left|\langle y \mid L\rangle \langle L \mid in\rangle\right|^2 = \text{probabilityof } |out\rangle = |y\rangle \text{ via } |L\rangle \\ P_y = \left|\langle y \mid in\rangle\right|^2 = \text{probabilityof } |out\rangle = |y\rangle \\ \text{ (independent of internal (unmeasurable properties))} \end{array}$$

Now

$$\begin{aligned} P_y &= \left|\langle y \mid in\rangle\right|^2 = \left|\langle y|\,\hat{I}\,|in\rangle\right|^2 = \left|\langle y|\left(|R\rangle\langle R| + |R\rangle\langle R|\right)|in\rangle\right|^2 \\ &= \left|\langle y \mid R\rangle \langle R \mid in\rangle + \langle y \mid L\rangle \langle L \mid in\rangle\right|^2 \end{aligned}$$

where

$$\begin{array}{l} \langle y \mid R\rangle \langle R \mid in\rangle = \text{ amplitude for } |out\rangle = |y\rangle \text{ via } |R\rangle \\ \langle y \mid L\rangle \langle L \mid in\rangle = \text{ amplitude for } |out\rangle = |y\rangle \text{ via } |L\rangle \end{array}$$

We then have

$$P_y = P_{Ry} + P_{Ly} + 2\text{Real}\left(\left(\langle y \mid R\rangle \langle R \mid in\rangle\right)^*\left(\langle y \mid L\rangle \langle L \mid in\rangle\right)\right)$$

Now,

$$\begin{array}{l} \langle y \mid R\rangle = \frac{i}{\sqrt{2}}\ ,\ \langle y \mid L\rangle = -\frac{i}{\sqrt{2}} \\ \langle R \mid in\rangle = \langle R|\,R(\theta)\,|x\rangle = e^{-i\theta}\langle R \mid x\rangle = \frac{1}{\sqrt{2}}e^{-i\theta} \\ \langle L \mid in\rangle = \langle L|\,R(\theta)\,|x\rangle = e^{i\theta}\langle L \mid x\rangle = \frac{1}{\sqrt{2}}e^{i\theta} \end{array}$$

so that

$$P_{Ry} = \frac{1}{4} = P_{Ly} \to P_{Ry} + P_{Ly} = \frac{1}{2} = \text{ classical probability result}$$

and

$$P_y = \frac{1}{4} + \frac{1}{4} + 2\text{Real}\left(\left(\frac{i}{\sqrt{2}}\frac{1}{\sqrt{2}}e^{-i\theta}\right)^* \left(-\frac{i}{\sqrt{2}}\frac{1}{\sqrt{2}}e^{i\theta}\right)\right) = \frac{1}{2}(1-\cos 2\theta)$$

is the quantum mechanical result. For $\theta = 30^\circ$ we have $P_y = 1/2 =$ quantum result, which is clearly different.

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

We have

$$\hat{\rho}_{in} = |in\rangle\langle in| \quad , \quad |in\rangle = \frac{\sqrt{3}}{2}|x\rangle + \frac{1}{2}|y\rangle = \frac{1}{2\sqrt{2}}\left((\sqrt{3}+i)|R\rangle + (\sqrt{3}-i)|L\rangle\right)$$

so that

$$\begin{aligned}\hat{\rho}_{in} &= \frac{3}{4}|x\rangle\langle x| + \frac{\sqrt{3}}{4}|x\rangle\langle y| + \frac{\sqrt{3}}{4}|y\rangle\langle x| + \frac{1}{4}|y\rangle\langle y| \\ &= \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{\sqrt{3}}{4}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \frac{\sqrt{3}}{4}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 3 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}_{xy}\end{aligned}$$

Since

$$Prob(j) = Tr(\hat{P}_j\hat{\rho}) = Tr(|j\rangle\langle j|\hat{\rho}) = \sum_k \langle k|(|j\rangle\langle j|\hat{\rho})|k\rangle = \sum_k \delta_{kj}\langle j|\hat{\rho}|k\rangle = \hat{\rho}_{jj}$$

we have

$$Prob(x) = \frac{3}{4} \quad , \quad Prob(y) = \frac{1}{4} = \text{ quantum result}$$

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

$$\frac{1}{4}\begin{pmatrix} 3 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}_{xy} \underset{measurement}{\rightarrow} \frac{1}{4}\begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}_{xy}$$

so that

$$Prob(x) = \frac{3}{4} \quad , \quad Prob(y) = \frac{1}{4} = \text{ as before}$$

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

$$\begin{aligned}\hat{\rho}_{in} &= \frac{1}{2}\left|R\right\rangle\left\langle R\right| + \frac{1+\sqrt{3}i}{8}\left|R\right\rangle\left\langle L\right| + \frac{1-\sqrt{3}i}{8}\left|L\right\rangle\left\langle R\right| + \frac{1}{2}\left|L\right\rangle\left\langle L\right| \\ &= \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1+\sqrt{3}i}{8}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \frac{1-\sqrt{3}i}{8}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \frac{1}{8}\begin{pmatrix} 4 & 1-\sqrt{3}i \\ 1+\sqrt{3}i & 4 \end{pmatrix}_{RL}\end{aligned}$$

which implies that

$$Prob(R) = \frac{1}{2} \quad , \quad Prob(L) = \frac{1}{2} = \text{ quantum result}$$

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

$$\hat{\rho}_{in} = \frac{1}{8}\begin{pmatrix} 4 & 1-\sqrt{3}i \\ 1+\sqrt{3}i & 4 \end{pmatrix}_{RL} \to \hat{\rho}_{out} = \frac{1}{8}\begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}_{RL}$$

Measurement has changed $\hat{\rho}_{out}$ to

$$\hat{\rho}_{out} = \frac{1}{2}\left|R\right\rangle\left\langle R\right| + \frac{1}{2}\left|L\right\rangle\left\langle L\right| \to \text{ a mixed state}$$

Changing back to the xy basis we get

$$\begin{aligned}\hat{\rho}_{out} &= \frac{1}{2}\frac{1}{2}\left(\left|x\right\rangle + i\left|y\right\rangle\right)\left(\left\langle x\right| - i\left\langle y\right|\right) + \frac{1}{2}\frac{1}{2}\left(\left|x\right\rangle - i\left|y\right\rangle\right)\left(\left\langle x\right| + i\left\langle y\right|\right) \\ &= \frac{1}{2}\left|x\right\rangle\left\langle x\right| + \frac{1}{2}\left|y\right\rangle\left\langle y\right| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_{xy} \to \text{ a mixed state}\end{aligned}$$

The density operator remains diagonal!

Clearly,

$$\Pr ob(x) = \frac{1}{2} \quad , \quad \Pr ob(y) = \frac{1}{2} = \text{ classical result}$$

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!

5.5.6 Photons and Polarizers

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

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

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

$$\langle x \mid \psi\rangle = \frac{i}{\sqrt{3}} \rightarrow P_y = |\langle x \mid \psi\rangle|^2 = \frac{1}{3}$$

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

$$\begin{aligned}
&|y'\rangle = -\sin\varphi\,|x\rangle + \cos\varphi\,|y\rangle \\
&\langle y' \mid \psi\rangle = -\sqrt{\tfrac{2}{3}}\sin\varphi + \tfrac{i}{\sqrt{3}}\cos\varphi \\
&P_{y'} = |\langle y' \mid \psi\rangle|^2 = \tfrac{2}{3}\sin^2\varphi + \tfrac{1}{3}\cos^2\varphi = \tfrac{1}{3}\left(2 - \cos^2\varphi\right)
\end{aligned}$$

(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.

$$\begin{aligned}
&|R\rangle = \tfrac{1}{\sqrt{2}}\left(|x\rangle + i\,|y\rangle\right) \rightarrow \langle R \mid \psi\rangle = \tfrac{1}{\sqrt{3}}\left(1 + \tfrac{\sqrt{2}}{2}\right) \\
&P_R = |\langle R \mid \psi\rangle|^2 = \tfrac{1}{2} + \tfrac{\sqrt{2}}{3} \rightarrow P_L = 1 - P_R = \tfrac{1}{2} - \tfrac{\sqrt{2}}{3}
\end{aligned}$$

The torque on the disk is the angular momentum transferred per second, which is

amount transferred by $|R\rangle$ per sec + amount transferred by $|L\rangle$ per sec

or

$$\begin{aligned}
&N\left(\hbar P(\hbar) - \hbar P(-\hbar)\right) \\
&N\left(\hbar P(R) - \hbar P(L)\right) \\
&N\hbar\left(\tfrac{1}{2} + \tfrac{\sqrt{2}}{3}\right) - N\hbar\left(\tfrac{1}{2} - \tfrac{\sqrt{2}}{3}\right) = \tfrac{2\sqrt{2}}{3}N\hbar
\end{aligned}$$

Thus, the torque is positive, which implies that the disk will rotate CCW as viewed from the positive $z-$axis.

5.5.7 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

$$\begin{pmatrix} 0 & -iE_0 \\ iE_0 & 0 \end{pmatrix} \begin{pmatrix} \langle x \mid E\rangle \\ \langle y \mid E\rangle \end{pmatrix} = E \begin{pmatrix} \langle x \mid E\rangle \\ \langle y \mid E\rangle \end{pmatrix}$$

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

$$\langle y \mid E_0\rangle = i\,\langle x \mid E_0\rangle \rightarrow |E_0\rangle = \frac{1}{\sqrt{2}}\left(|x\rangle + i\,|y\rangle\right) = |R\rangle$$

and for $E = -E_0$, we get

$$\langle y \mid -E_0\rangle = -i\,\langle x \mid -E_0\rangle \rightarrow |-E_0\rangle = \frac{1}{\sqrt{2}}\left(|x\rangle - i\,|y\rangle\right) = |L\rangle$$

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

$$|\psi(0)\rangle = |in\rangle = |x\rangle = |E_0\rangle\,\langle E_0 \mid x\rangle + |-E_0\rangle\,\langle -E_0 \mid x\rangle = \frac{1}{\sqrt{2}}\left(|E_0\rangle + |-E_0\rangle\right)$$

This implies that

$$\begin{aligned} |out\rangle &= e^{-i\hat{H}t/\hbar}\,|in\rangle = e^{-i\hat{H}t/\hbar}\frac{1}{\sqrt{2}}\left(|E_0\rangle + |-E_0\rangle\right) = \frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}\,|E_0\rangle + e^{iE_0t/\hbar}\,|-E_0\rangle\right) \\ &= \cos\left(\frac{E_0t}{\hbar}\right)|x\rangle + \sin\left(\frac{E_0t}{\hbar}\right)|y\rangle = |\psi(t)\rangle \end{aligned}$$

(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.

5.5.8 K-Meson oscillations

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

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

where

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

and

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

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

Before the absorber we have the state

$$|\psi_{before}\rangle = |K_L\rangle = \frac{1}{\sqrt{2}}\left(\left|K^0\right\rangle - \left|\bar{K}^0\right\rangle\right)$$

The effect of the thin absorber is expressed by the development operator

$$\hat{A} = \left|K^0\right\rangle\left\langle K^0\right| e^{i\theta} + \left|\bar{K}^0\right\rangle\left\langle \bar{K}^0\right| e^{i(\theta+\pi/18)}$$

so that only the relative phase of the components is changed by $10^\circ = \pi/18$. Therefore, after the absorber the state is

$$|\psi_{after}\rangle = \hat{A}\,|\psi_{before}\rangle = \frac{e^{i\theta}}{\sqrt{2}}\left(\left|K^0\right\rangle - e^{i\pi/18}\left|\bar{K}^0\right\rangle\right)$$

We know the time dependence of the $|K_L\rangle, |K_S\rangle$ states so we now rewrite this state in that basis

$$\begin{aligned}|\psi_{after}\rangle &= \frac{e^{i\theta}}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}(|K_S\rangle + |K_L\rangle) - e^{i\pi/18}\frac{1}{\sqrt{2}}(|K_S\rangle - |K_L\rangle)\right) \\ &= \frac{e^{i\theta}}{2}\left(\left(1 - e^{i\pi/18}\right)|K_S\rangle + \left(1 + e^{i\pi/18}\right)|K_L\rangle\right)\end{aligned}$$

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)

$$\begin{aligned}|K_L(t)\rangle &= e^{-i\omega_L t - t/2\tau_L}|K_L\rangle \\ |K_S(t)\rangle &= e^{-i\omega_S t - t/2\tau_S}|K_S\rangle\end{aligned}$$

Therefore, for $t > 0$, we have

$$|\psi(t)\rangle = \frac{e^{i\theta}}{2}\left(\left(1 - e^{i\pi/18}\right)e^{-i\omega_S t - t/2\tau_S}|K_S\rangle + \left(1 + e^{i\pi/18}\right)e^{-i\omega_L t - t/2\tau_L}|K_L\rangle\right)$$

The probability amplitude for observing $|K_S\rangle$ for $t > 0$ is

$$\langle K_S \mid \psi(t)\rangle = \frac{e^{i\theta}}{2}\left(1 - e^{i\pi/18}\right)e^{-i\omega_S t - t/2\tau_S}$$

and the corresponding probability is

$$P_S = |\langle K_S \mid \psi(t)\rangle|^2 = \frac{1}{2}\left(1 - \cos\frac{\pi}{18}\right)e^{-t/\tau_S}$$

Note that for $\pi/18 \to 0$ or no relative phase shift, the probability $= 0$, that is, the beam stays all $|K_L\rangle$ as it should.

Now we have

$$\begin{aligned}&d = 5\,cm \to t_d = \tfrac{d}{v} \approx \tfrac{d}{c} = 1.6\times 10^{-10}\text{ sec} \\ &\tau_S = 0.9\times 10^{-10}\text{ sec} \to \tfrac{t_d}{\tau_S} = \tfrac{16}{9}\end{aligned}$$

Now the number of transitions per sec at time t is given by $N(0)P_S(t)$. This says that the

$$\text{total number of transitions}(0 \to t_d) = \bar{N} = \int_0^{t_d} N(0)P_S(t)dt$$

$$\bar{N} = \frac{1}{2}\left(1 - \cos\frac{\pi}{18}\right)N(0)\int_0^{t_d} e^{-t/\tau_S}dt = \frac{1}{2}\left(1 - \cos\frac{\pi}{18}\right)\tau_S N(0)(1 - e^{-16/9}) = 0.0063\tau_S N(0)$$

where we assumed $N(0) =$ constant since the total number of decays is very small compared to $N(0)$. Therefore,

$$\text{fraction } = \frac{\bar{N}}{N(0)} = 0.0063\tau_S = 5.69\times 10^{-13}$$

5.5.9 What comes out?

A beam of spin 1/2 particles is sent through series of three Stern-Gerlach measuring devices as shown in Figure 5.1 below: The first SGz device transmits

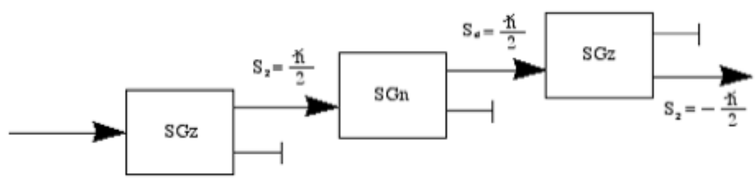


Figure 5.1: Stern-Gerlach Setup

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

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

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 $\left|\pm\hat{z}\right\rangle$. The first measurement corresponds to the projection operator

$$\hat{M}(+\hat{z}) = \left|+\hat{z}\right\rangle\left\langle+\hat{z}\right|$$

The second measurement is given by the projection operator

$$\hat{M}(+\hat{n}) = \left|+\hat{n}\right\rangle\left\langle+\hat{n}\right|$$

where

$$\left|+\hat{n}\right\rangle = \cos\frac{\theta}{2}\left|+\hat{z}\right\rangle + \sin\frac{\theta}{2}\left|-\hat{z}\right\rangle$$

so that

$$\hat{M}(+\hat{n}) = \cos^2\frac{\theta}{2}\left|+\hat{z}\right\rangle\left\langle+\hat{z}\right| + \cos\frac{\theta}{2}\sin\frac{\theta}{2}\left(\left|+\hat{z}\right\rangle\left\langle-\hat{z}\right| + \left|-\hat{z}\right\rangle\left\langle+\hat{z}\right|\right) + \sin^2\frac{\theta}{2}\left|-\hat{z}\right\rangle\left\langle-\hat{z}\right|$$

The last measurement corresponds to the projection operator

$$\hat{M}(-\hat{z}) = \left|-\hat{z}\right\rangle\left\langle-\hat{z}\right|$$

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

This is maximized by choosing $\theta = \pi/2$ so that $f_{max} = 1/4$.

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

If there is no third device, then the fraction surviving is

$$\begin{aligned}\bar{f} &= \left| \langle +\hat{n}| \hat{M}(+\hat{n}) |+\hat{z}\rangle \right|^2 = \left| \langle +\hat{n}| (\cos^2\frac{\theta}{2} + \cos\frac{\theta}{2}\sin\frac{\theta}{2}) |+\hat{z}\rangle \right|^2 \\ &= \left| \cos^3\frac{\theta}{2} + \cos^2\frac{\theta}{2}\sin\frac{\theta}{2} \right|^2 = \cos^4\frac{\theta}{2}(1+\sin 2\theta)\end{aligned}$$

5.5.10 Orientations

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

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

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

For a general linearly polarized state at angle θ 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

$$\cos\theta = -\frac{1}{2} \quad , \quad \sin\theta = -\frac{\sqrt{3}}{2}$$

or $\theta = 210° = -150°$.

For

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

we have

$$\cos\theta = -\frac{1}{2} \quad , \quad \sin\theta = +\frac{\sqrt{3}}{2}$$

or $\theta = 330° = -30°$.

For

$$|\psi_2\rangle = |h\rangle$$

we have

$$\cos\theta = 1 \quad , \quad \sin\theta = 0$$

or $\theta = 0°$.

5.5.11 Find the phase angle

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

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

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

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

and $\tau_L \gg \tau_S$.

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

We have

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

where A is the normalization factor. We then have

$$\begin{aligned}\langle K'_L \mid K'_L\rangle &= |A_L|^2\left[(1+\varepsilon^*)\left\langle K^0\right| - (1-\varepsilon^*)\left\langle \bar{K}^0\right|\right]\left[(1+\varepsilon)\left|K^0\right\rangle - (1-\varepsilon)\left|\bar{K}^0\right\rangle\right] \\ &= 2\,|A_L|^2\left(1+|\varepsilon|^2\right) = 1\end{aligned}$$

or

$$A_L = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}$$

Now we must also have

$$\langle K'_S \mid K'_S\rangle = 1 \quad , \quad \langle K'_S \mid K'_L\rangle = 0$$

We assume that

$$|K_L'\rangle = \left[a\left|K^0\right\rangle + b\left|\bar{K}^0\right\rangle\right]$$

and we get

$$|a|^2 + |b|^2 = 1 \quad , \quad a^*(1+\varepsilon) - b^*(1-\varepsilon) = 0$$

If we choose

$$a = \frac{1-\varepsilon^*}{\sqrt{2(1+|\varepsilon|^2)}} \quad , \quad b = \frac{1+\varepsilon^*}{\sqrt{2(1+|\varepsilon|^2)}}$$

then both the conditions are satisfied so that

$$\begin{aligned} |K_L'\rangle &= \tfrac{1}{\sqrt{2(1+|\varepsilon|^2)}}\left[(1+\varepsilon)\left|K^0\right\rangle - (1-\varepsilon)\left|\bar{K}^0\right\rangle\right] \\ |K_S'\rangle &= \tfrac{1}{\sqrt{2(1+|\varepsilon|^2)}}\left[(1-\varepsilon^*)\left|K^0\right\rangle + (1+\varepsilon^*)\left|\bar{K}^0\right\rangle\right] \end{aligned}$$

or rewriting in the $(|K_L\rangle, |K_S\rangle)$ basis we have

$$\begin{aligned} |K_L'\rangle &= \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}\left[(1+\varepsilon)\frac{1}{\sqrt{2}}(|K_L\rangle + |K_S\rangle) - (1-\varepsilon)\frac{1}{\sqrt{2}}(|K_S\rangle - |K_L\rangle)\right] \\ &= \frac{1}{\sqrt{(1+|\varepsilon|^2)}}(|K_L\rangle + \varepsilon|K_S\rangle) \end{aligned}$$

$$\begin{aligned} |K_S'\rangle &= \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}\left[(1-\varepsilon^*)\frac{1}{\sqrt{2}}(|K_L\rangle + |K_S\rangle) + (1+\varepsilon^*)\frac{1}{\sqrt{2}}(|K_S\rangle - |K_L\rangle)\right] \\ &= \frac{1}{\sqrt{(1+|\varepsilon|^2)}}(|K_S\rangle - \varepsilon^*|K_L\rangle) \end{aligned}$$

and

$$\begin{aligned} |K_L'(t)\rangle &= \tfrac{1}{\sqrt{(1+|\varepsilon|^2)}}\left(e^{-i\omega_L t - t/2\tau_L}|K_L\rangle + \varepsilon e^{-i\omega_S t - t/2\tau_S}|K_S\rangle\right) \\ |K_S'(t)\rangle &= \tfrac{1}{\sqrt{(1+|\varepsilon|^2)}}\left(e^{-i\omega_S t - t/2\tau_S}|K_S\rangle - \varepsilon^* e^{-i\omega_L t - t/2\tau_L}|K_L\rangle\right) \end{aligned}$$

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

We are interested in the ratio

$$R = \frac{|\langle CP = +1 \mid K_L'(t)\rangle|^2}{|\langle CP = -1 \mid K_S'(t)\rangle|^2} = \frac{|\langle K_S \mid K_L'(t)\rangle|^2}{|\langle K_S \mid K_S'(t)\rangle|^2}$$

Notice that if $|K'_L\rangle \to |K_L\rangle$, 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

$$R = \frac{|\langle K_S \mid K'_L(t)\rangle|^2}{|\langle K_S \mid K'_S(t)\rangle|^2} = \frac{\frac{1}{\sqrt{(1+|\varepsilon|^2)}} \left|\varepsilon^2\right| e^{-t/\tau_L}}{\frac{1}{\sqrt{(1+|\varepsilon|^2)}} e^{-t/\tau_S}} = |\varepsilon|^2 e^{t(1/\tau_S - 1/\tau_L)}$$

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 δ. Derive an expression for the number of two pion events observed as a function of time of travel from the absorber. How well would such a measurement (given δ) enable one to determine the phase of ε?

The number of two pion events ($CP = -1$) is proportional to the probability

$$P_{K'_L \to K_S}(t) = |\langle K_S \mid K'_L(t)\rangle|^2$$

so we will calculate that quantity.

We have before the asorber

$$|\psi_{before}\rangle = |K'_L\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}} \left[(1+\varepsilon)\left|K^0\right\rangle - (1-\varepsilon)\left|\bar{K}^0\right\rangle\right]$$

and after the absorber

$$\begin{aligned}
|\psi_{after}\rangle = |\psi(0)\rangle &= \frac{1}{\sqrt{2(1+|\varepsilon|^2)}} \left[(1+\varepsilon)\left|K^0\right\rangle - e^{-i\delta}(1-\varepsilon)\left|\bar{K}^0\right\rangle\right] \\
&= \frac{1}{\sqrt{2(1+|\varepsilon|^2)}} \left[(1+\varepsilon)\frac{1}{\sqrt{2}}(|K_L\rangle + |K_S\rangle) - e^{-i\delta}(1-\varepsilon)\frac{1}{\sqrt{2}}(|K_S\rangle - |K_L\rangle)\right] \\
&= \frac{1}{2\sqrt{(1+|\varepsilon|^2)}} \left[\left((1+\varepsilon) - e^{-i\delta}(1-\varepsilon)\right)|K_S\rangle + \left((1+\varepsilon) + e^{-i\delta}(1-\varepsilon)\right)|K_L\rangle\right]
\end{aligned}$$

so that

$$|K'_L(t)\rangle = \frac{1}{2\sqrt{(1+|\varepsilon|^2)}} \left[\begin{array}{l} \left((1+\varepsilon) - e^{-i\delta}(1-\varepsilon)\right) e^{-i\omega_S t - t/2\tau_S}|K_S\rangle \\ \quad + \left((1+\varepsilon) + e^{-i\delta}(1-\varepsilon)\right) e^{-i\omega_L t - t/2\tau_L}|K_L\rangle \end{array}\right]$$

and

$$P_{K'_L \to K_S}(t) = |\langle K_S \mid K'_L(t)\rangle|^2 = \frac{1}{4(1+|\varepsilon|^2)} \left|(1+\varepsilon) - e^{-i\delta}(1-\varepsilon)\right|^2 e^{-t/\tau_S}$$

This is the probability of two pion events as a function of time.

Now

$$\begin{aligned}
&\left|(1+\varepsilon)-e^{-i\delta}(1-\varepsilon)\right|^2 = \left((1+\varepsilon^*)-e^{i\delta}(1-\varepsilon^*)\right)\left((1+\varepsilon)-e^{-i\delta}(1-\varepsilon)\right) \\
&= (1+\varepsilon^*)(1+\varepsilon)+(1-\varepsilon^*)(1-\varepsilon)-(1+\varepsilon^*)(1-\varepsilon)e^{-i\delta}-(1-\varepsilon^*)(1+\varepsilon)e^{i\delta} \\
&= 1+\varepsilon^*+\varepsilon+|\varepsilon|^2+1-\varepsilon^*-\varepsilon+|\varepsilon|^2-\left(1+\varepsilon^*-\varepsilon-|\varepsilon|^2\right)e^{-i\delta}-\left(1-\varepsilon^*+\varepsilon-|\varepsilon|^2\right)e^{i\delta} \\
&= 2+2|\varepsilon|^2-2\left(1-|\varepsilon|^2\right)\cos\delta+2i(\varepsilon^*-\varepsilon)\sin\delta \\
&= 2(1-\cos\delta)+2|\varepsilon|^2(1+\cos\delta)+2\mathrm{Im}(\varepsilon)\sin\delta
\end{aligned}$$

so that

$$P_{K_L'\to K_S}(t) = \frac{1}{(1+|\varepsilon|^2)}\left((1-\cos\delta)+|\varepsilon|^2(1+\cos\delta)+\mathrm{Im}(\varepsilon)\sin\delta\right)e^{-t/\tau_S}$$

Now measuring $R \to |\varepsilon|$ and then measuring $P_{K_L'\to K_S}(t) \to \mathrm{Im}(\varepsilon)$. We then have

$$\mathrm{Re}(\varepsilon) = \sqrt{|\varepsilon|^2-(\mathrm{Im}(\varepsilon))^2} \to phase(\varepsilon) = \varphi = \tan^{-1}\frac{\mathrm{Re}(\varepsilon)}{\mathrm{Im}(\varepsilon)} = \tan^{-1}\frac{\sqrt{|\varepsilon|^2-(\mathrm{Im}(\varepsilon))^2}}{\mathrm{Im}(\varepsilon)}$$

5.5.12 Quarter-wave plate

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

We have for a quarter-wave plate

$$\hat{Q} = |x\rangle\langle x| + e^{i\pi/2}|y\rangle\langle y| \to \text{ changes relative phase by } \pi/2$$

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

$$\langle R\,|\,out\rangle = \frac{1}{\sqrt{2}}(\langle x| - i\langle y|)\left(\frac{\sqrt{2}}{2}|x\rangle + \frac{i}{2}|y\rangle\right) = \frac{\sqrt{3}+1}{2\sqrt{2}}$$

$$P_R = |\,\langle R\,|\,out\rangle\,|^{\frac{2+\sqrt{3}}{4}}$$

$$BraketL|out = \frac{1}{\sqrt{2}}(\langle x| + i\,\langle y|)\left(\frac{\sqrt{2}}{2}\,|x\rangle + \frac{i}{2}\,|y\rangle\right) = \frac{-\sqrt{3}+1}{2\sqrt{2}}$$

$$P_L = |\,\langle L\,|\,out\rangle\,|^{\frac{2-\sqrt{3}}{4}}$$

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.

5.5.13 What is happening?

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

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

Photons exiting the last polaroid are in the state $|y'(\varphi)\rangle$, polarized at angle φ 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 $\langle x \mid y \rangle = 0$.

For $\varphi = 90°$, ($|y'\rangle = |x\rangle$), the total probability is not equal to $|\langle x \mid y \rangle|^2 = 0$, 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!!

5.5.14 Interference

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

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

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

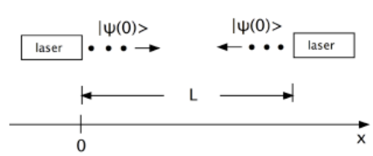


Figure 5.2: Interference Setup

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

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

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

$$\begin{aligned}
P(x) &= |\langle\psi(t) \mid \psi(t)\rangle|^2 = |e^{-2piix/\lambda} + e^{-2pii(L-x)/\lambda}|^2 |\langle\psi(0) \mid \psi(0)\rangle|^2 \\
&= |e^{-2piix/\lambda} + e^{-2piiL/\lambda} e^{2piix/\lambda}|^2 \\
&= |e^{piiL/\lambda} e^{-2piix/\lambda} + e^{-piiL/\lambda} e^{2piix/\lambda}|^2 \\
&= |e^{2pii(x-L/2)/\lambda} + e^{-2pii(x-L/2)/\lambda}|^2 \\
&= 4\cos^2\left(\frac{2\pi}{\lambda}\left(x - \frac{L}{2}\right)\right)
\end{aligned}$$

(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.

5.5.15 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.

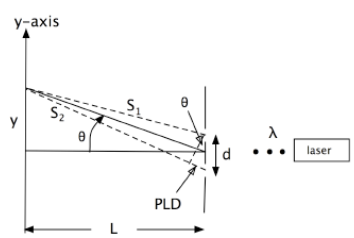


Figure 5.3: Double-Slit Interference Setup

We calculate PLD as follows:

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

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

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

Using the result of 7.5.14 we have

$$|screen\ at\ y\rangle = |\psi(y)\rangle = e^{-i2\pi S_1/\lambda}\,|\psi_0\rangle + e^{-i2\pi S_2/\lambda}\,|\psi_0\rangle$$

Thus, the probability of detection at y is

$$|\langle\psi(y)\,|\,\psi(y)\rangle|^2 = |e^{-i2\pi S_1/\lambda} + e^{-i2\pi S_2/\lambda}|^2\ vert\,\langle\psi_0\,|\,\psi_0\rangle|^2$$

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

$$P(y) = 4\cos^2\left(\frac{\pi(S_2-S_1)}{\lambda}\right) = 4\cos^2\left(\frac{\pi y d}{\lambda L}\right)$$

5.5.16 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).

Figure 5.4: 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.

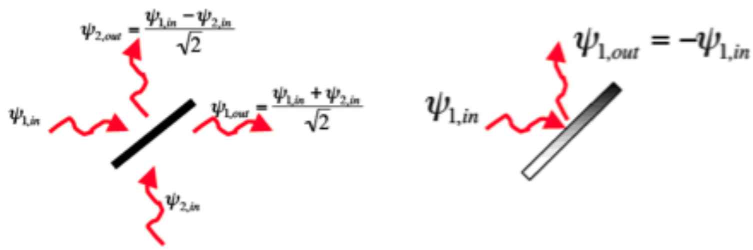
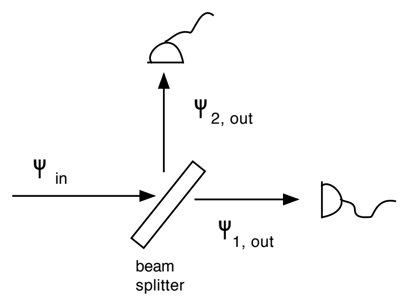


Figure 5.5: Input-Output transformation

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

We have



According to the rules given

$$\psi_{1,out} = \frac{1}{\sqrt{2}}\psi_{in} \quad , \quad \psi_{2,out} = \frac{1}{\sqrt{2}}\psi_{in}$$

since nothing enters part #2. By the Born rule, the probability to find a photon a position 1 or 2 is

$$P_{1,out} = \int |\psi_{1,out}|^2 dx = \frac{1}{2}\int |\psi_{in}|^2 dx = \frac{1}{2}$$

$$P_{2,out} = \int |\psi_{2,out}|^2 dx = \frac{1}{2}\int |\psi_{in}|^2 dx = \frac{1}{2}$$

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):

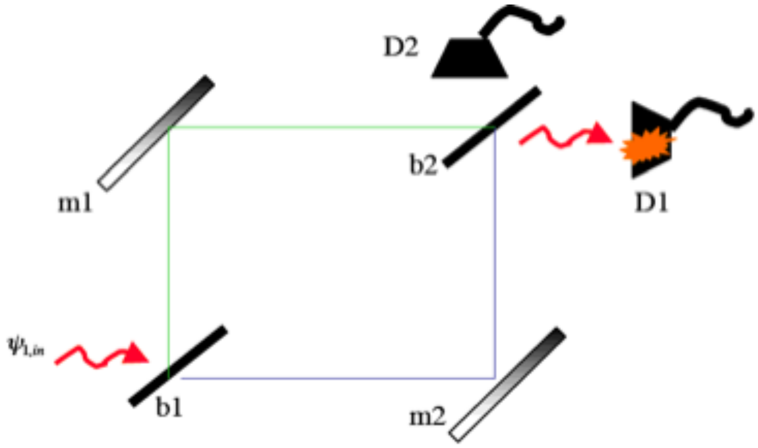


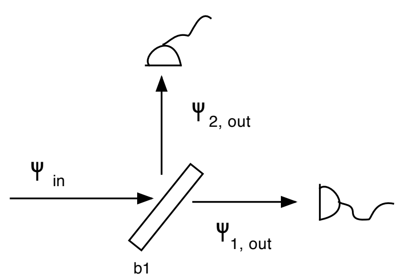
Figure 5.6: Input-Output transformation

The wave is split at beam-splitter b1, where it travels either path b1-m1-b2(call it the green path) or the path b1-m2-b2 (call it the blue path). Mirrors are then used to recombine the beams on a second beam splitter, b2. Detectors D1 and D2 are placed at the two output ports of b2.

Assuming the paths are perfectly balanced (that is equal length), show that the probability for detector D1 to click is 100% - *no randomness*!

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.

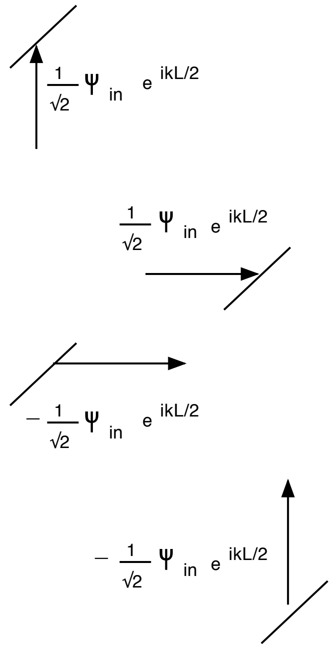
Beam splitter #1:



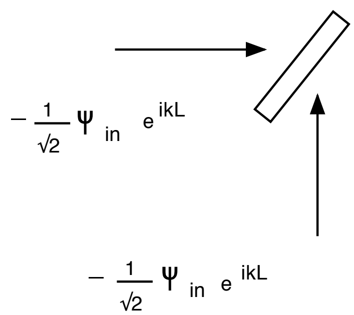
Propagation a distance $L/2$:

$$\rightarrow phase \;\; e^{ikL/2}$$

Bounce off mirrors:

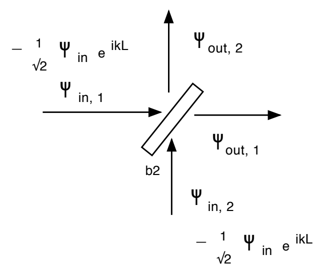


Another propagation by a distance $L/2$:



$$\rightarrow phase \;\; e^{ikL}$$

Beam splitter #2:



where

$$\psi_{out,1} = \frac{\psi_{in,1} + \psi_{in,2}}{\sqrt{2}} = e^{ikL}\psi_{in}$$

$$\psi_{out,2} = \frac{\psi_{in,1} - \psi_{in,2}}{\sqrt{2}} = 0$$

Therefore,

$$P_{out,1} = \int dx|\psi_{out,1}|^2 = \int dx|\psi_{in}|^2 = 1$$

$$P_{out,2} = \int dx|\psi_{out,2}|^2 = 0$$

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

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

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

$$P(blue) = P(green) = \frac{1}{2}$$

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

$$P(transmission\ at\ b2|green\ path) = P(reflection\ at\ b2|blue\ path) = \frac{1}{2}$$

Therefore

$$P_{D1} = \frac{1}{2}\frac{1}{2} + \frac{1}{2}\frac{1}{2} = \frac{1}{2}$$

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.,

$$\psi_{total} = \frac{\frac{1}{\sqrt{2}}\psi_{in}e^{ikL} + \frac{1}{\sqrt{2}}\psi_{in}e^{ikL}}{\sqrt{2}}$$

so that

$$P_{D1} = \int dx|\psi_{total}|^2 = \frac{1}{2}\frac{1}{2} + \frac{1}{2}\frac{1}{2} + \frac{1}{2}\frac{1}{2} + \frac{1}{2}\frac{1}{2} = 1$$

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

$$\psi_{1,out} = \frac{\frac{1}{\sqrt{2}}\psi_{in}e^{ikL+\Delta L} + \frac{1}{\sqrt{2}}\psi_{in}e^{ikL}}{\sqrt{2}}$$

$$\psi_{2,out} = \frac{\frac{1}{\sqrt{2}}\psi_{in}e^{ikL+\Delta L} - \frac{1}{\sqrt{2}}\psi_{in}e^{ikL}}{\sqrt{2}}$$

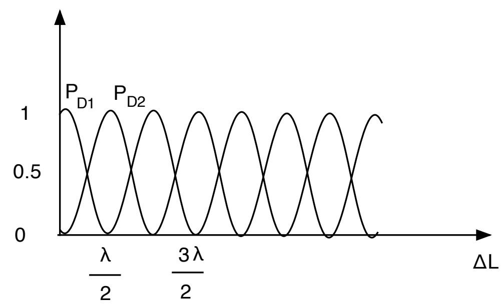
We then have

$$\begin{aligned}
P_{D1} &= \int dx|\psi_{1,out}|^2 = \frac{1}{4}\int dx|\psi_{in}e^{ikL+\Delta L} + \psi_{in}e^{ikL}|^2 \\
&= \frac{1}{4}\int dx|\psi_{in}|^2|e^{ikL}|^2|e^{ik\Delta L} + 1|^2 \\
&= \frac{1}{4}(e^{ik\Delta L} + 1)(e^{-ik\Delta L} + 1) = \frac{1 + \cos(k\Delta L)}{2} \\
&= \cos^2\left(\frac{k\Delta L}{2}\right)
\end{aligned}$$

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 ΔL look like



These are the *interference fringes* associated with this interferometer.

5.5.17 More Mach-Zender

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

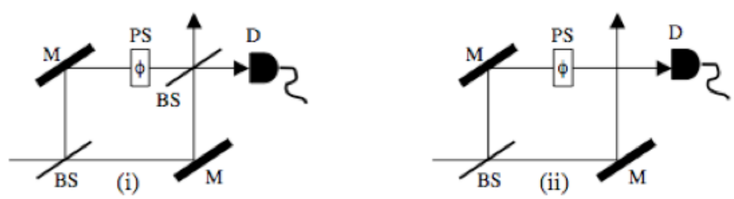


Figure 5.7: Mach-Zender Setups

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

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

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 6

Schrodinger Wave equation
1-Dimensional Quantum Systems

6.15 Problems

6.15.1 Delta function in a well

A particle of mass m moving in one dimension is confined to a space $0 < x < L$ by an infinite well potential. In addition, the particle experiences a delta function potential of strength λ given by $\lambda\delta(x - L/2)$ located at the center of the well as shown in Figure 6.1 below.

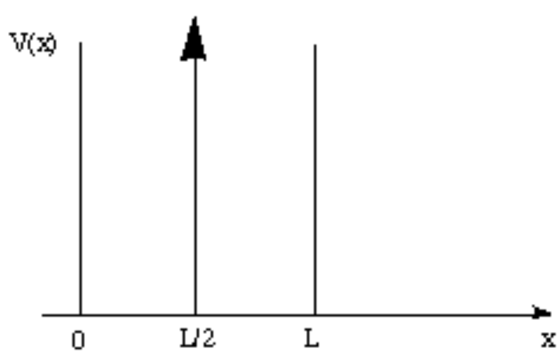


Figure 6.1: Potential Diagram

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

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

$$\psi_I(x=L/2) = \psi_{II}(x=L/2) \to A_1 = A_2$$

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

$$-A_1 k\cos\frac{kL}{2} - A_1 k\cos\frac{kL}{2} = \frac{2m\lambda}{\hbar^2}\sin\frac{kL}{2} \to \tan\frac{kL}{2} = -\frac{\hbar^2}{m\lambda}k$$

Therefore, we have a transcendental equation for

$$k \to E = \frac{\hbar^2 k^2}{2m}$$

6.15.2 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

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \quad , \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad , \; n = 1,2,3,.....$$

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

$$\begin{aligned}\psi(x,t=0) &= \sqrt{\frac{8}{5a}}\left(1+\cos\left(\frac{\pi x}{a}\right)\right)\sin\left(\frac{\pi x}{a}\right) \\ &= \sqrt{\frac{8}{5a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{5a}}\sin\left(\frac{2\pi x}{a}\right) \\ &= \sqrt{\frac{4}{5}}\psi_1(x) + \sqrt{\frac{1}{5}}\psi_2(x)\end{aligned}$$

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

$$\psi(x,t_0) = \sqrt{\frac{4}{5}} e^{-iE_1t_0/\hbar}\psi_1(x) + \sqrt{\frac{1}{5}} e^{-iE_2t_0/\hbar}\psi_2(x)$$

(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

$$|\psi(x,t_0|^2 = e^{-iE_1t_0/\hbar} \left| e^{-iE_1t_0/\hbar} \sqrt{\frac{8}{5a}} \sin\left(\frac{\pi x}{a}\right) \left(1 + \cos\left(\frac{\pi x}{a}\right) e^{-i(E_2-E_1)t_0/\hbar}\right) \right|^2$$
$$= \frac{8}{5a}\sin^2\left(\frac{\pi x}{a}\right)\left(1 + \cos^2\left(\frac{\pi x}{a}\right) + 2\cos\left(\frac{\pi x}{a}\right)\cos\frac{3\pi^2\hbar^2}{2ma^2}t_0\right)$$

so that

$$P(0 \leq x \leq a/2; t_0) = \frac{1}{2} + \frac{16}{15\pi}\cos\frac{3\pi^2\hbar^2}{2ma^2}t_0$$

6.15.3 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

$$\kappa^2 = \frac{2m\,|E|}{\hbar^2} \quad , \quad q^2 = \frac{2m(|E| + V_0)}{\hbar^2} \quad , \quad \beta^2 = \frac{2mV_0}{\hbar^2}$$

The Schrodinger equation is

$$\begin{array}{ll} \psi'' = \kappa^2\psi & |x| > a \\ \psi'' = q^2\psi & |x| < a \end{array}$$

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

$$\psi(x) = \begin{cases} Ae^{-\kappa|x|} & |x| > a \\ Be^{q|x|} + Ce^{-q|x|} & |x| < a \end{cases}$$

Continuity at $x = a$ and $x = 0$ leads to the condition (eigenvalue equation)

$$e^{2qa}\left(\frac{1 - g^2/2q}{1 + g^2/2q}\right) = \frac{q - \kappa}{q + \kappa}$$

In the case of vanishing V_0, we recover the equation

$$E_0 = -\frac{\hbar^2}{2m}\left(\frac{g^2}{2}\right)^2$$

appropriate 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

$$\xi = qa \quad , \quad \lambda = \frac{g^2 a}{2} \quad , \quad b = \beta a$$

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.

6.15.4 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

$$k=\sqrt{\frac{2mE}{\hbar}} \quad , \quad q=\sqrt{\frac{2m(E-V)}{\hbar}}$$

Continuity of the wave function at $x = 0$ gives

$$1+B=C$$

Integrating the Schrodinger equation over the infinitesimal interval around the origin gives

$$\begin{array}{c} -\frac{\hbar^2}{2m}\left(\psi'(0+)-\psi'(0-)\right)=\frac{\hbar^2 g}{2m}\psi(0) \\ 1-B=-\frac{i}{k}(g+iq)C \end{array}$$

From the two relationships between B and C we obtain

$$\begin{array}{c} C=\frac{2}{1+q/k-ig/k} \\ B=\frac{1-q/k+ig/k}{1+q/k-ig/k} \end{array}$$

The reflection coefficient is

$$\Re=\left|\frac{j_r}{j_l}\right|=\frac{(\hbar k/m)\left|B\right|^2}{\hbar k/m}=\left|\frac{1-q/k+ig/k}{1+q/k-ig/k}\right|^2=\frac{(1-q/k)^2+g^2/k^2}{(1+q/k)^2+g^2/k^2}$$

In the high energy limit we have

$$\Re = \frac{g\hbar^2}{8mE}$$

For the pure step barrier we have (in the same limit)

$$\Re = \frac{V^2}{8E^2}$$

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

$$\kappa_- = \sqrt{\frac{2m\,|E|}{\hbar^2}} \quad , \quad \kappa_+ = \sqrt{\frac{2m(V + |E|)}{\hbar^2}}$$

Then we can write the bound-state wave function as

$$\psi(x) = \begin{cases} Ae^{\kappa_- x} & x < 0 \\ Ae^{-\kappa_+ x} & x > 0 \end{cases}$$

The discontinuity at the origin implies that

$$\begin{aligned} &-\tfrac{\hbar^2}{2m}(-A\kappa_+ - A\kappa_-) = \tfrac{\hbar^2 g}{2m} A \\ &\kappa_+ + \kappa_- = g \end{aligned}$$

This then gives

$$E = -\frac{m}{2\hbar^2 g^2}\left(\frac{\hbar^2 g^2}{2m} - V\right)^2$$

and

$$\kappa_\pm^2 = \frac{m^2}{\hbar^4 g^2}\left(\frac{\hbar^2 g^2}{2m} \pm V\right)^2$$

and

$$A = \sqrt{\frac{2\kappa_+\kappa_-}{g}}$$

6.15.5 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 6.2 below.

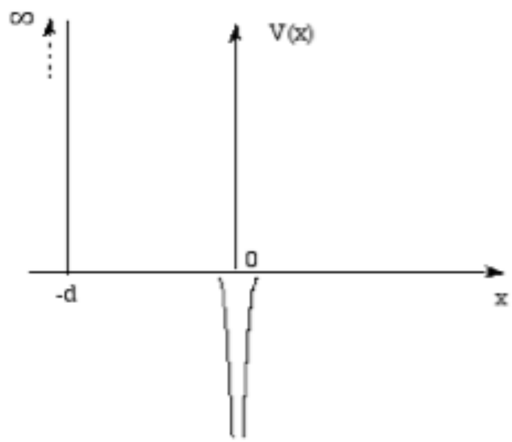


Figure 6.2: Potential Diagram

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

For $x > -d$, the Schrodinger equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E + V_0\delta(x)\right)\psi = 0$$

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 Schrodinger equation across the discontinuity we find

$$\lim_{\varepsilon\to 0}\left[\int_{-\varepsilon}^{\varepsilon}\frac{d^2\psi}{dx^2}dx + \frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}E\psi(x)dx + \frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}V_0\delta(x)\psi(x)dx\right] = 0$$
$$0 = \Delta\left(\frac{d\psi}{dx}\right) + \frac{2mV_0}{\hbar^2}\psi(0) \to \psi_2'(0) - \psi_1'(0) = -\frac{2mV_0}{\hbar^2}\psi_2(0)$$
$$-k - k(a-b) = -\frac{2mV_0}{\hbar^2}$$

At $x = -d$, we have an infinite well, so that $\psi_1(-d) = 0$ or

$$\begin{array}{l} a + b = 1 \\ -k - k(a-b) = -\frac{2mV_0}{\hbar^2} \\ ae^{-kd} + be^{kd} = 0 \end{array}$$

with solutions

$$a = -\frac{e^{2kd}}{1-e^{2kd}} \quad , \quad b = \frac{1}{1-e^{2kd}} \quad , \quad k = \frac{mV_0}{\hbar^2}\left(1 - e^{-2kd}\right)$$

(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 1^{st}-order result by inserting the 0^{th}-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

$$\begin{aligned} E = -\frac{\hbar^2 k^{(1)2}}{2m} &\approx -\frac{\hbar^2}{2m}\left(\frac{mV_0}{\hbar^2}\right)^2\left(1 - e^{-2\frac{mV_0}{\hbar^2}d}\right)^2 \\ &\approx -\frac{mV_0^2}{2\hbar^2}\left(1 - 2e^{-2\frac{mV_0}{\hbar^2}d}\right) \\ &= -\frac{mV_0^2}{2\hbar^2} + \frac{mV_0^2}{\hbar^2}e^{-2\frac{mV_0}{\hbar^2}d} \end{aligned}$$

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

$$\frac{2mV_0 d}{\hbar^2} = 2k^{(0)}d \approx 2kd << 1 \to d > \frac{1}{k} \approx \frac{1}{k^{(0)}} = \frac{\hbar^2}{mV_0}$$

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

$$k = \frac{mV_0}{\hbar^2}\left(1 - e^{-2kd}\right)$$

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

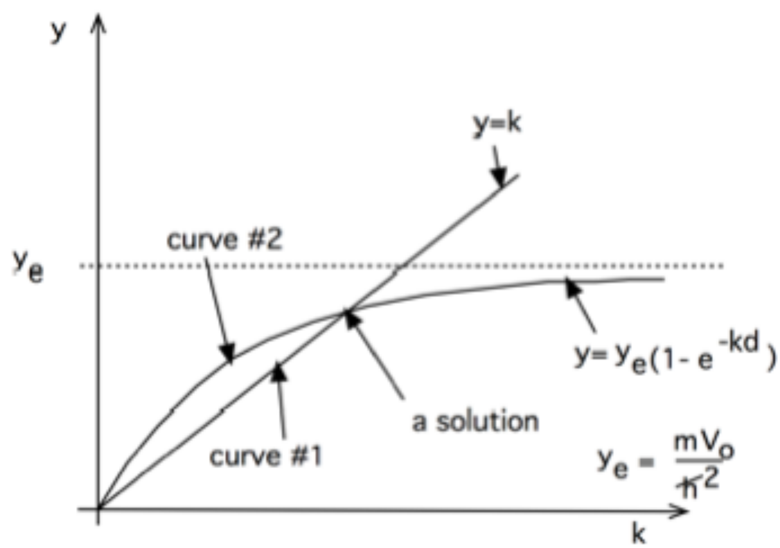


Figure 6.3: Staircase Function

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 grater than the slope of curve #1 (the straight line).

Now

$$\left.\frac{dy_1}{dk}\right|_{k=0} = 1 \quad and \quad \left.\frac{dy_2}{dk}\right|_{k=0} = \frac{2mVd_0}{\hbar^2}$$

Therefore, if

$$V_0 d > \frac{\hbar^2}{2m}$$

then there exists at least one bound state.

6.15.6 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

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad , \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad , n = 1, 2, 3, ...$$

We then have

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n \psi_n(x) e^{-iE_n t/\hbar}$$

We evaluate the a_n coefficients using the initial wavefunction

$$\begin{aligned} &\psi(x,0) = \sum_{n=1}^{\infty} a_n \psi_n(x) \\ &\int_0^a \psi(x,0)\psi_k(x)dx = \sum_{n=1}^{\infty} a_n \int_0^a \psi_n(x)\psi_k(x)dx = \sum_{n=1}^{\infty} a_n \delta_{nk} = a_k \end{aligned}$$

so that

$$a_k = \int_0^a \psi(x,0)\psi_k(x)dx = \frac{2}{a}\int_0^{a/2} \sin \frac{k\pi x}{a} dx = \frac{2}{k\pi}\left(1 - \cos \frac{k\pi}{2}\right)$$

Therefore,

$$\psi(x,t) = \frac{2}{\pi}\sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} \frac{1}{n}\left(1 - \cos \frac{n\pi}{2}\right) \sin \frac{n\pi x}{a} e^{-i\frac{n^2\pi^2\hbar}{2ma^2}t}$$

(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!

6.15.7 $1/x$ 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 Schrodinger 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 Schrodinger 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 $\lim_{x\to\infty} f(x_e^{-ax} \to 0$. Substituting into the Schrodinger equation we get

$$\left(f''(x) - 2\alpha f'(x) + \frac{me^2}{2\hbar^2 x} f(x)\right) e^{-\alpha x} = 0 \to f''(x) - 2\alpha f'(x) + \frac{me^2}{2\hbar^2 x} f(x) = 0$$

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 sate since it has zeroes only at the boundaries ($x = 0$ and $x \to \infty$). We find A by

$$1 = A^2 \int_0^\infty |\psi(x)|^2 dx = A^2 \int_0^\infty x^2 e^{-2\alpha x} dx = \frac{A^2}{8\alpha^3} \int_0^\infty y^2 e^{-y} dy = \frac{A^2}{8\alpha^3} \Gamma(3) = \frac{A^2}{4\alpha^3} \to A = 2\alpha^{3/2}$$

(d) Find the ground state energy.

$$E_0 = -\frac{\hbar^2 \alpha^2}{2m} = -\frac{me^4}{32\hbar^2} = -\frac{e^2}{8a_0} = \frac{1}{4} E_{hydrogen}^{ground-state}$$

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

We then have

$$\begin{aligned}
\langle \psi | \hat{x} | \psi \rangle &= \int_0^\infty \int_0^\infty \langle \psi \mid x' \rangle \langle x' | \hat{x} | x \rangle \langle x \mid \psi \rangle \, dx dx' = \int_0^\infty \int_0^\infty \langle \psi \mid x' \rangle x \delta(x - x') \langle x \mid \psi \rangle \, dx dx' \\
&= \int_0^\infty \langle \psi \mid x \rangle \, x \, \langle x \mid \psi \rangle \, dx = \int_0^\infty x \, |\psi(x)|^2 \, dx = A^2 \int_0^\infty x^3 e^{-2\alpha x} dx \\
&= \frac{4\alpha^3}{(2\alpha)^4} \Gamma(4) = \frac{3}{2\alpha} = 6a_0
\end{aligned}$$

6.15.8 Using the commutator

Using the coordinate-momentum commutation relation prove that

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

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

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

Since

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

we have

$$\left[\hat{H}, \hat{x}\right] = \frac{1}{2m}\left[\hat{p}^2, \hat{x}\right] = -\frac{i\hbar\hat{p}}{m}$$

and so

$$\left[\left[\hat{H}, \hat{x}\right], \hat{x}\right] = -\frac{i\hbar}{m}\left[\hat{p}, \hat{x}\right] = -\frac{\hbar^2}{m}$$

Therefore,

$$\langle E_m| \left[\left[\hat{H}, \hat{x}\right], \hat{x}\right] |E_m\rangle = -\frac{\hbar^2}{m}$$

On the other hand, we also have (using $\hat{H}|E_m\rangle = E_m|E_m\rangle$)

$$\langle E_m| \left[\left[\hat{H}, \hat{x}\right], \hat{x}\right] |E_m\rangle = \langle E_m| \left(\hat{H}\hat{x}^2 - 2\hat{x}\hat{H}\hat{x} - \hat{x}^2\hat{H}\right) |E_m\rangle = 2E_m \langle E_m| \hat{x}^2 |E_m\rangle - 2\langle E_m| \hat{x}\hat{H}\hat{x} |E_m\rangle$$

and

$$\langle E_m| \hat{x}^2 |E_m\rangle = \sum_n \langle E_m| \hat{x} |E_n\rangle \langle E_n| \hat{x} |E_m\rangle = \sum_n |\langle E_m| \hat{x} |E_n\rangle|^2$$

$$\langle E_m| \hat{x}\hat{H}\hat{x} |E_m\rangle = \sum_n \langle E_m| \hat{x}\hat{H} |E_n\rangle \langle E_n| \hat{x} |E_m\rangle = \sum_n E_n \langle E_m| \hat{x} |E_n\rangle \langle E_n| \hat{x} |E_m\rangle = \sum_n E_n |\langle E_m| \hat{x} |E_n\rangle|^2$$

Therefore,

$$\begin{aligned}
-\frac{\hbar^2}{m} &= \langle E_m| \left[\left[\hat{H}, \hat{x}\right], \hat{x}\right] |E_m\rangle = 2E_m \langle E_m| \hat{x}^2 |E_m\rangle - 2\langle E_m| \hat{x}\hat{H}\hat{x} |E_m\rangle \\
&= 2E_m \sum_n |\langle E_m| \hat{x} |E_n\rangle|^2 - 2\sum_n E_n |\langle E_m| \hat{x} |E_n\rangle|^2
\end{aligned}$$

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

$$\sum_n (E_n - E_0) |\langle E_0| \hat{x} |E_n\rangle|^2 = \frac{\hbar^2}{2m}$$

6.15.9 Matrix Elements for Harmonic Oscillator

Compute the following matrix elements

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

We have

$$\begin{aligned} &\hat{x} = x_0(\hat{a}+\hat{a}^+) \quad , \quad x_0 = \sqrt{\tfrac{\hbar}{2m\omega}} \\ &\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \quad , \quad \hat{a}^+\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \end{aligned}$$

We then have

$$\langle n'|\,\hat{x}\,|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\langle n'|\,\hat{a}\,|n\rangle + \langle n'|\,\hat{a}^+\,|n\rangle\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right)$$

From this result we get

$$\begin{aligned} \langle n'|\,\hat{x}^2\,|n\rangle &= \sum_m \langle n'|\,\hat{x}\,|m\rangle\,\langle m|\,\hat{x}\,|n\rangle \\ &= \tfrac{\hbar}{2m\omega}\sum_m\left(\sqrt{m}\delta_{n',m-1} + \sqrt{m+1}\delta_{n',m+1}\right)\left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right) \\ &= \tfrac{\hbar}{2m\omega}\left(\sqrt{n(n-1)}\delta_{n',n-2} + \sqrt{(n+1)(n+2)}\delta_{n',n+2} + (2n+1)\delta_{n',n}\right) \end{aligned}$$

$$\begin{aligned} \langle n'|\,\hat{x}^3\,|n\rangle &= \sum_m \langle n'|\,\hat{x}^2\,|m\rangle\,\langle m|\,\hat{x}\,|n\rangle \\ &= \left(\tfrac{\hbar}{2m\omega}\right)^{3/2}\sum_m\left(\sqrt{m(m-1)}\delta_{n',m-2} + \sqrt{(m+1)(m+2)}\delta_{n',m+2} + (2m+1)\delta_{n',m}\right) \\ &\times\left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right) \\ &= \left(\tfrac{\hbar}{2m\omega}\right)^{3/2}\left(\begin{array}{l} \sqrt{n(n-1)(n-2)}\delta_{n',n-3} + 3n\sqrt{n}\delta_{n',n-1} \\ \quad +(3n+3)\sqrt{n+1}\delta_{n',n+1} + \sqrt{(n+1)(n+2)(n+3)}\delta_{n',n+3} \end{array}\right) \end{aligned}$$

$$\begin{aligned} \langle n'|\,\hat{x}^4\,|n\rangle &= \sum_m \langle n'|\,\hat{x}^2\,|m\rangle\,\langle m|\,\hat{x}^2\,|n\rangle \\ &= \left(\tfrac{\hbar}{2m\omega}\right)^2\sum_m\left(\begin{array}{l} \sqrt{m(m-1)}\delta_{n',m-2} \\ \quad +\sqrt{(m+1)(m+2)}\delta_{n',m+2} + (2m+1)\delta_{n',m} \end{array}\right) \\ &\times\left(\begin{array}{l} \sqrt{n(n-1)}\delta_{m,n-2} \\ \quad +\sqrt{(n+1)(n+2)}\delta_{m,n+2} + (2n+1)\delta_{m,n} \end{array}\right) \\ &\left(\tfrac{\hbar}{2m\omega}\right)^2\left(\begin{array}{l} \sqrt{n(n-1)(n-2)(n-3)}\delta_{n',n-4} \\ \quad +2(2n-1)\sqrt{n(n-1)}\delta_{n',n-2} + 3(2n^2+2n+1)\delta_{n',n} \\ \quad +4(n+1)\sqrt{(n+1)(n+2)}\delta_{n',n+2} \\ \quad +\sqrt{(n+1)(n+2)(n+3)(n+4)}\delta_{n',n+4} \end{array}\right) \end{aligned}$$

We then have

$$\hat{p} = -i\sqrt{\frac{m\hbar\omega_0}{2}}\left(\hat{a}-\hat{a}^+\right)$$

and thus

$$\begin{aligned} \langle n'|\,\hat{p}\,|n\rangle &= -i\sqrt{\frac{m\hbar\omega_0}{2}}\left(\langle n'|\,\hat{a}\,|n\rangle - \langle n'|\,\hat{a}^+\,|n\rangle\right) \\ &= -i\sqrt{\frac{m\hbar\omega_0}{2}}\left(\sqrt{n}\delta_{n',n-1} - \sqrt{n+1}\delta_{n',n+1}\right) \end{aligned}$$

so that

$$\begin{aligned}
&\langle n'|\,\hat{x}\hat{p}\,|n\rangle = \sum_m \langle n'|\,\hat{x}\,|m\rangle\,\langle m|\,p\,|n\rangle = \\
&-\tfrac{i\hbar}{2}\sum_m \left(\sqrt{m}\delta_{n',m-1} + \sqrt{m+1}\delta_{n',m+1}\right)\left(\sqrt{n}\delta_{m,n-1} - \sqrt{n+1}\delta_{m,n+1}\right) \\
&= -\tfrac{i\hbar}{2}\left(\sqrt{n(n-1)}\delta_{n',n-2} - \sqrt{(n+1)(n+2)}\delta_{n',n+2} - 1)\delta_{n',n}\right)
\end{aligned}$$

6.15.10 A matrix element

Show for the one dimensional simple harmonic oscillator

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

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

We want to evaluate

$$\langle 0|\,e^{ik\hat{x}}\,|0\rangle = \sum_{n=0}^{\infty}\frac{(ik)^n}{n!}\,\langle 0|\,\hat{x}^n\,|0\rangle$$

Now

$$\begin{aligned}
&\langle 0|\,\hat{x}^0\,|0\rangle = \langle 0\mid 0\rangle = 1 \\
&\langle 0|\,\hat{x}\,|0\rangle = \sqrt{\tfrac{\hbar}{2m\omega}}\,\langle 0|\,(\hat{a}+\hat{a}^+)\,|0\rangle = 0 \to \langle 0|\,\hat{x}^n\,|0\rangle = 0 \quad n\ odd \\
&\langle 0|\,\hat{x}^2\,|0\rangle = \tfrac{\hbar}{2m\omega}\,\langle 0|\,(\hat{a}+\hat{a}^+)^2\,|0\rangle = \tfrac{\hbar}{2m\omega}\,\langle 0|\,\hat{a}\hat{a}^+\,|0\rangle = \tfrac{\hbar}{2m\omega} \\
&\langle 0|\,\hat{x}^4\,|0\rangle = \tfrac{\hbar}{2m\omega}\,\langle 0|\,(\hat{a}\hat{a}\hat{a}^+\hat{a}^+ + \hat{a}\hat{a}^+\hat{a}\hat{a}^+)\,|0\rangle = 3\left(\tfrac{\hbar}{2m\omega}\right)^2 \\
&\langle 0|\,\hat{x}^6\,|0\rangle = 15\left(\tfrac{\hbar}{2m\omega}\right)^3 \quad , \quad \langle 0|\,\hat{x}^8\,|0\rangle = 105\left(\tfrac{\hbar}{2m\omega}\right)^4 \\
&\langle 0|\,\hat{x}^{2n}\,|0\rangle = \left(\prod_{\substack{j\le 2n \\ j\ odd}} j\right)\left(\tfrac{\hbar}{2m\omega}\right)^n = \tfrac{(2n)!}{2^n n!}\left(\tfrac{\hbar}{2m\omega}\right)^n
\end{aligned}$$

Therefore

$$\begin{aligned}
\langle 0|\,e^{ik\hat{x}}\,|0\rangle &= \sum_{n=0}^{\infty}\frac{(ik)^n}{n!}\,\langle 0|\,\hat{x}^n\,|0\rangle = 1 - \frac{k^2}{2!}\,\langle 0|\,\hat{x}^2\,|0\rangle + \frac{k^4}{4!}\,\langle 0|\,\hat{x}^4\,|0\rangle - \frac{k^6}{6!}\,\langle 0|\,\hat{x}^6\,|0\rangle + ... \\
&= 1 - \frac{k^2}{2!}\frac{\hbar}{2m\omega} + \frac{k^4}{4!}3\left(\frac{\hbar}{2m\omega}\right)^2 - \frac{k^6}{6!}15\left(\frac{\hbar}{2m\omega}\right)^3 + ... \\
&= 1 - \frac{1}{1!}\frac{k^2}{2}\,\langle 0|\,\hat{x}^2\,|0\rangle + \frac{1}{2!}\left(\frac{k^2}{2}\,\langle 0|\,\hat{x}^2\,|0\rangle\right)^2 - \frac{1}{3!}\left(\frac{k^2}{2}\,\langle 0|\,\hat{x}^2\,|0\rangle\right)^3 + ... \\
&= e^{-\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle}
\end{aligned}$$

Alternatively, we can use the result

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

to get

$$\langle 0| e^{ik\hat{x}} |0\rangle = e^{\frac{\hbar k^2}{4m\omega}} \langle 0| e^{ik\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}+\hat{a}^+\right)} |0\rangle = e^{\frac{\hbar k^2}{4m\omega}} \langle 0| e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}} e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}^+} |0\rangle$$

Now expanding the exponential operators we have

$$\begin{aligned}\langle 0| e^{ik\hat{x}} |0\rangle &= e^{\frac{\hbar k^2}{4m\omega}} \langle 0| \left(1 + ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a} + \frac{1}{2}\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^2 \hat{a}^2 + ...\right) \\ &\quad \times \left(1 + ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}^+ + \frac{1}{2}\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^2 \hat{a}^{+\,2} + ...\right) \\ &= e^{\frac{\hbar k^2}{4m\omega}} \left(1 - \frac{k^2\hbar}{2m\omega} + \frac{k^4\hbar^2}{8m^2\omega^2} - ....\right) = e^{\frac{\hbar k^2}{4m\omega}} e^{-\frac{\hbar k^2}{2m\omega}} = e^{-\frac{\hbar k^2}{4m\omega}}\end{aligned}$$

Since

$$\langle 0| \hat{x}^2 |0\rangle = \frac{\hbar}{2m\omega}$$

we have

$$\langle 0| e^{ik\hat{x}} |0\rangle = e^{-\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle}$$

as above.

6.15.11 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

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}(t) + \hat{a}^+(t)\right)$$

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 $\hat{H} = \hbar\omega(\hat{a}^+\hat{a} + 1/2)$. Using the result of an earlier problem we have

$$\hat{a}(t) = e^{i\hat{H}t/\hbar}\hat{a}e^{-i\hat{H}t/\hbar} = \hat{a} + \frac{it}{\hbar}\left[\hat{H},\hat{a}\right] + \frac{1}{2}\left(\frac{it}{\hbar}\right)^2\left[\hat{H},\left[\hat{H},\hat{a}\right]\right] + ...$$

Now

$$\left[\hat{H},\hat{a}\right] = \hbar\omega\left[\hat{a}^+\hat{a},\hat{a}\right] = \hbar\omega\left(\hat{a}^+\hat{a}\hat{a} - \hat{a}\hat{a}^+\hat{a}\right) = -\hbar\omega\hat{a}$$

so that

$$\hat{a}(t) = \hat{a} - i\omega t\hat{a} + \frac{1}{2}(i\omega t)^2 \hat{a} - \frac{1}{6}(i\omega t)^3 \hat{a} + ... = e^{-i\omega t}\hat{a}$$

and similarly,

$$\hat{a}^+(t) = e^{i\omega t}\hat{a}^+$$

so that

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}}\left(e^{-i\omega t}\hat{a} + e^{i\omega t}\hat{a}^+\right)$$

In the same way we find that

$$\hat{p}(t) = i\sqrt{\frac{\hbar m\omega}{2}}\left(e^{i\omega t}\hat{a}^+ - e^{-i\omega t}\hat{a}\right)$$

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

$$\begin{aligned} C(t) &= \langle 0|\,\hat{x}(t)\hat{x}(0)\,|0\rangle \\ &= \langle 0|\sqrt{\frac{\hbar}{2m\omega}}\left(e^{-i\omega t}\hat{a} + e^{i\omega t}\hat{a}^+\right)\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^+\right)|0\rangle \\ &= \frac{\hbar}{2m\omega}\left(e^{-i\omega t}\langle 0|\,\hat{a}\hat{a}^+\,|0\rangle\right) = \frac{\hbar}{2m\omega}e^{-i\omega t} \end{aligned}$$

All other terms are zero since

$$\langle 0|\,\hat{a}\hat{a}\,|0\rangle = 0 = \langle 0|\,\hat{a}^+\hat{a}\,|0\rangle = \langle 0|\,\hat{a}^+\hat{a}^+\,|0\rangle$$

6.15.12 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

$$P(0) = |\langle 0 \mid \psi\rangle|^2 = \left|\langle 0|\,e^{-ip_0 x/\hbar}\,|0\rangle\right|^2$$

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,

$$e^{-ip_0 x/\hbar} = e^{-ip_0\sqrt{\frac{\hbar}{2m\omega}}(a^+ + a)/\hbar} = e^{-ip_0\sqrt{\frac{\hbar}{2m\omega}}a^+/\hbar} e^{-ip_0\sqrt{\frac{\hbar}{2m\omega}}a/\hbar} e^{-p_0^2/4m\hbar\omega}$$

Therefore, we have

$$P(0) = e^{-p_0^2/2m\hbar\omega}\left|\langle 0| e^{-ip_0\sqrt{\frac{\hbar}{2m\omega}}a^+/\hbar} e^{-ip_0\sqrt{\frac{\hbar}{2m\omega}}a/\hbar} |0\rangle\right|^2 = e^{-p_0^2/2m\hbar\omega} \left|\langle 0 \mid 0\rangle\right|^2 = e^{-p_0^2/2m\hbar\omega}$$

where we have used

$$e^{-ip_0\sqrt{\frac{\hbar}{2m\omega}}a/\hbar} |0\rangle = |0\rangle \quad , \quad \langle 0| e^{-ip_0\sqrt{\frac{\hbar}{2m\omega}}a^+/\hbar} = \langle 0|$$

6.15.13 Coherent States

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

We have

$$|z\rangle = e^{z\hat{a}^+} |0\rangle$$

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

$$\begin{aligned}
\hat{a} |z\rangle = \hat{a} e^{z\hat{a}^+} |0\rangle &= \sum_{n=0}^{\infty} \frac{z^n}{n!} \hat{a}(\hat{a}^+)^n |0\rangle = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \hat{a} \left(\frac{(\hat{a}^+)^n}{\sqrt{n!}} |0\rangle\right) \\
&= \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \hat{a} |n\rangle = \sum_{n=1}^{\infty} \frac{z^n}{\sqrt{n!}} \sqrt{n} |n-1\rangle = z \sum_{n=1}^{\infty} \frac{z^{n-1}}{\sqrt{(n-1)!}} |n-1\rangle \\
&= z \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle = z \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \left(\frac{(\hat{a}^+)^n}{\sqrt{n!}} |0\rangle\right) = z e^{z\hat{a}^+} |0\rangle = z |z\rangle
\end{aligned}$$

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

$$\begin{aligned}
\langle z_1 \mid z_2\rangle = \langle 0| e^{z*_1 a^+} e^{z_2 \hat{a}^+} |0\rangle &= \left(\sum_{m=0}^{\infty} \frac{z*_1^m}{\sqrt{m!}} \langle m|\right) \left(\sum_{n=0}^{\infty} \frac{z_2^n}{\sqrt{n!}} |n\rangle\right) \\
&= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{z_2^n}{\sqrt{n!}} \frac{z*_1^m}{\sqrt{m!}} \langle m \mid n\rangle = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{z_2^n}{\sqrt{n!}} \frac{z*_1^m}{\sqrt{m!}} \delta_{mn} \\
&= \sum_{n=0}^{\infty} \frac{z_2^n}{\sqrt{n!}} \frac{z*_1^n}{\sqrt{n!}} = \sum_{n=0}^{\infty} \frac{z_2^n z*_1^n}{n!} = e^{z*_1 z_2}
\end{aligned}$$

(c) Show that the completeness relation takes the form

$$\begin{aligned}\int \frac{dxdy}{\pi} |z\rangle \langle z| e^{-z^* z} &= \int \frac{dxdy}{\pi} e^{z\hat{a}^+} |0\rangle \langle 0| e^{z^* \hat{a}} e^{-z^* z} \\ &= \sum_{m,n} \int \frac{dxdy}{\pi} \frac{z^m (\hat{a}^+)^m}{m!} |0\rangle \langle 0| \frac{(z*)^n (\hat{a})^n}{n!} e^{-z^* z} \\ &= \sum_{m,n} \int_0^{2\pi} \frac{d\varphi}{\pi} \int_0^{\infty} rdr \frac{r^m e^{im\varphi} (\hat{a}^+)^m}{m!} |0\rangle \langle 0| \frac{r^n e^{-in\varphi} (\hat{a})^n}{n!} e^{-r^2}\end{aligned}$$

where we have used $z = re^{i\varphi}$. Now

$$\int_0^{2\pi} \frac{d\varphi}{\pi} e^{i(m-n)\varphi} = 2\delta_{mn}$$

Therefore, doing the m sum we have

$$\begin{aligned}\int \frac{dxdy}{\pi} |z\rangle \langle z| e^{-z^* z} &= \sum_n \frac{1}{n!} \int_0^{\infty} r r^{2n} e^{-r^2} dr \left(\frac{(\hat{a}^+)^n}{\sqrt{n!}} |0\rangle \right) \left(\langle 0| \frac{(\hat{a})^n}{\sqrt{n!}} \right) \\ &= \sum_n \frac{1}{n!} \int_0^{\infty} r r^{2n} e^{-r^2} dr \left(|n\rangle\right) \left(\langle n|\right) = \sum_n |n\rangle \langle n| \frac{1}{n!} \int_0^{\infty} r r^{2n} e^{-r^2} dr\end{aligned}$$

Now using $r^2 = x$ we have

$$\int_0^{\infty} r r^{2n} e^{-r^2} dr = \int_0^{\infty} x^n e^{-x} dx = n!$$

so that

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

This unusual form of the completeness relation reflects the fact that the coherent states form an *overcomplete* set of states.

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

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

6.15.14 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 $\psi(o)\delta(x)$, 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

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{2\nu}(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi_{2\nu}(x) = E_{2\nu}\psi_{2\nu}(x) = \hbar\omega(2\nu + 1/2)\psi_{2\nu}(x)$$

The new Schrodinger equation is then

$$-\tfrac{\hbar^2}{2m}\tfrac{d^2\psi_E(x)}{dx^2} + \tfrac{1}{2}m\omega^2 x^2\psi_E(x) - E\psi_E(x) = -\tfrac{\hbar^2 g}{2m}\psi_E(0)\delta(x)$$
$$\sum_{\nu=0}^{\infty} C_{2\nu}\left(-\tfrac{\hbar^2}{2m}\tfrac{d^2}{dx^2} + \tfrac{1}{2}m\omega^2 x^2 - E\right)\psi_{2\nu}(x) = -\tfrac{\hbar^2 g}{2m}\psi_E(0)\delta(x)$$
$$\sum_{\nu=0}^{\infty} C_{2\nu}\left(\hbar\omega\left(2\nu + \tfrac{1}{2}\right) - E\right)\psi_{2\nu'}(x) = -\tfrac{\hbar^2 g}{2m}\psi_E(0)\delta(x)$$

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

$$\psi_E(x) = \sum_{\nu=0}^{\infty} C_{2\nu}\psi_{2\nu}(x) = -\frac{\hbar^2 g}{2m}\psi_E(0) \sum_{\nu=0}^{\infty} \frac{\psi_{2\nu}(0)}{\hbar\omega\left(2\nu + \frac{1}{2}\right) - E}\psi_{2\nu}(x)$$

At the point $x = 0$, this expression is true provided that

$$\frac{1}{g} = -\frac{\hbar^2}{2m} \sum_{\nu=0}^{\infty} \frac{|\psi_{2\nu}(0)|^2}{\hbar\omega\left(2\nu + \frac{1}{2}\right) - E}$$

Using the given values of $\psi_{2\nu}(0)$, this is equivalent to

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

(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

$$\frac{4}{g} = -\sqrt{\frac{\hbar}{m\omega}} \frac{\Gamma(1/4 - E/2\hbar\omega)}{\Gamma(3/4 - E/2\hbar\omega)}$$

The right-hand side has poles at the points

$$\frac{1}{4} - \frac{E}{2\hbar\omega} = -n \quad , \quad n = 0, 1, 2, ... \Rightarrow E = \hbar\omega\left(2n + \frac{1}{2}\right)$$

and zeroes at the points

$$\frac{3}{4} - \frac{E}{2\hbar\omega} = -n \quad , \quad n = 0, 1, 2, ... \Rightarrow E = \hbar\omega\left(2n + \frac{3}{2}\right)$$

$$\Gamma(z) = \frac{\Gamma(z+1)}{z}$$

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.

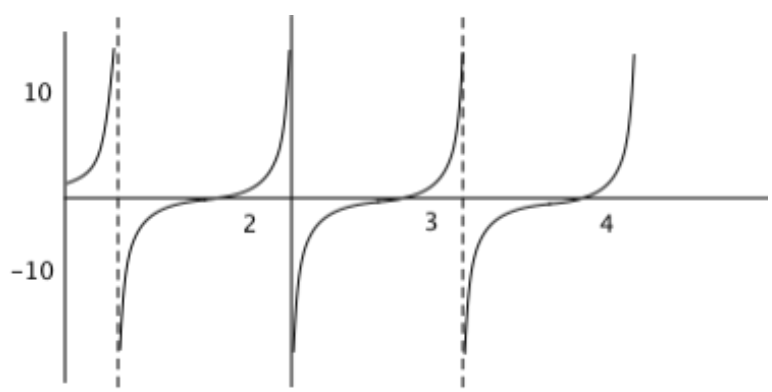


Figure 6.4: Plot of $\frac{\Gamma(1/4-x)}{\Gamma(3/4-x)}$

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

$$-\frac{4}{g}\sqrt{\frac{m\omega}{\hbar}} = \frac{\Gamma(1/4 + |E|/2\hbar\omega)}{\Gamma(3/4 + |E|/2\hbar\omega)}$$

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

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

6.15.15 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

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{a}}\cos\left(\frac{\pi x}{a}\right) & |x| \le a/2 \\ 0 & |x| \ge a/2 \end{cases}$$

The possible values one can measure for any observable are its eigenvalues, say α, with probability

$$P_\alpha = |\langle\alpha \mid \psi\rangle|^2$$

(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

$$\tilde{\psi}(k) = \langle u_k \mid \psi\rangle = \int\limits_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}e^{-ikx}\psi(x)$$

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

$$\psi(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{\pi x}{a}\right)\theta(x) \quad all\ x \quad where \quad \theta(x) = \left\{ \begin{array}{l} 1\,|x| \leq a/2 \\ 0\,|x| \geq a/2 \end{array} \right.$$

Method #1: Fourier Transform

Using the first form of the wave function we get

$$\tilde{\psi}(k) = \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx = \sqrt{\frac{2}{a}} \int_{-a/2}^{a/2} \cos\left(\frac{\pi x}{a}\right) e^{-ikx} dx = \frac{1}{2}\sqrt{\frac{2}{a}} \int_{-a/2}^{a/2} \left(e^{i\pi x/a} + e^{-i\pi x/a}\right) e^{-ikx} dx$$

$$= \frac{1}{2}\sqrt{\frac{2}{a}} \int_{-a/2}^{a/2} \left(e^{i(\pi/a-k)x} + e^{-i(\pi/a+k)x}\right) dx$$

$$= \frac{1}{2}\sqrt{\frac{2}{a}} \frac{1}{i(\pi/a-k)} \int_{-i(\pi/a-k)a/2}^{i(\pi/a-k)a/2} e^{y} dy + \frac{1}{2}\sqrt{\frac{2}{a}} \frac{1}{-i(\pi/a+k)} \int_{i(\pi/a+k)a/2}^{-i(\pi/a+k)a/2} e^{y} dy$$

$$= \frac{1}{2}\sqrt{\frac{2}{a}} \frac{-2i\sin(\pi/a-k)a/2}{i(\pi/a-k)} + \frac{1}{2}\sqrt{\frac{2}{a}} \frac{-2i\sin(\pi/a+k)a/2}{-i(\pi/a+k)}$$

$$= \sqrt{\frac{a}{2}} \left[Sinc\left(\frac{ka}{2} - \frac{\pi}{2}\right) + Sinc\left(\frac{ka}{2} - \frac{\pi}{2}\right)\right]$$

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

$$\tilde{A}(k) = \tilde{B}(k) * \tilde{C}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq \tilde{B}(q) \tilde{C}(k-q)$$

We have to find

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

where

$$\psi(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right) \theta(x)$$

Defining

$$B(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right)$$

we have

$$\tilde{B}(k) = \int_{-\infty}^{\infty} \sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right) e^{-ikx} dx = \frac{1}{2}\sqrt{\frac{2}{a}} \int_{-\infty}^{\infty} \left(e^{i\pi x/a} + e^{-i\pi x/a}\right) e^{-ikx} dx$$

$$= \frac{1}{2}\sqrt{\frac{2}{a}} \sqrt{2\pi} \left[\delta(k - \pi/a) + \delta(k + \pi/a)\right]$$

These two delta functions correspond to a *standing wave* which is the superposition of $e^{ip_1 x/\hbar}$ and $e^{-ip_1 x/\hbar}$ where $p_1 = \pi/a$.

Now defining

$$C(x) = \theta(x)$$

we have

$$\tilde{C}(k) = \int_{-\infty}^{\infty} \theta(x) e^{-ikx} dx = \int_{-a/2}^{a/2} e^{-ikx} dx = \frac{2}{k} \sin\frac{ka}{2} = aSinc\left(\frac{ka}{2}\right)$$

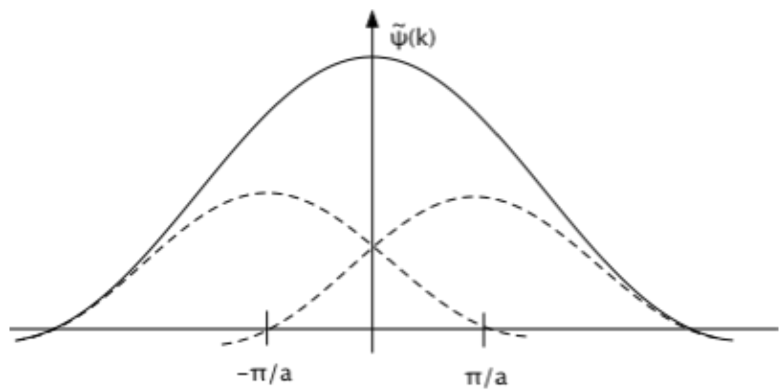
and then we have

$$\tilde{A}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq \tilde{B}(q) \tilde{C}(k - q)$$

$$= \frac{1}{\sqrt{2\pi}} \frac{a}{2} \sqrt{\frac{2}{a}} \sqrt{2\pi} \int_{-\infty}^{\infty} dq \left[\delta(q - \pi/a) + \delta(q + \pi/a)\right] Sinc\left(\frac{(k - q)a}{2}\right)$$

$$= \sqrt{\frac{a}{2}} \left[Sinc\left(\frac{ka}{2} - \frac{\pi}{2}\right) + Sinc\left(\frac{ka}{2} - \frac{\pi}{2}\right)\right] = \tilde{\psi}(k)$$

which is the same as the first result. This looks like



The dotted curves are the two 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

$$\tilde{\varphi}(p) = \frac{1}{\sqrt{\hbar}}\tilde{\psi}(k = p/\hbar)$$

we have any value $-\infty < p < +\infty$ where the probability density is

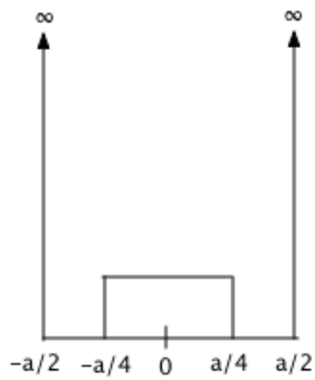
$$P(p) = |\tilde{\varphi}(p)|^2$$

(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

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

and so

$$c_n = \int dx \, u_n^*(x) \psi_+(x) = \langle u_n \mid \psi_+ \rangle$$

Since $\psi_+(x)$ is an even function, only the cosine terms survive. Thus, for $n = 1, 3, 5, ...$

$$c_n = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \int_{-a/4}^{a/4} \cos\frac{n\pi x}{a} dx = \frac{2}{n\pi}\left(\sin\frac{n\pi}{4} - \sin\frac{-n\pi}{4}\right) = \frac{4}{n\pi}\sin\frac{n\pi}{4} \quad n = 1, 3, 5, 7, ...$$

and therefore, the possible energies are

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2ma^2} \quad n = 1, 3, 5, ...$$

with probability

$$|c_n|^2 = \frac{16}{n^2\pi^2}\sin^2\frac{n\pi}{4} = \frac{8}{n^2\pi^2} \quad n = 1,3,5,7,.....$$

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

$$\tilde{\varphi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi_+(x)e^{-ipx/\hbar}dx$$

This implies that

$$\tilde{\varphi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{2}{a}}\int_{-\infty}^{\infty}e^{-ipx/\hbar}dx = \frac{1}{\sqrt{\pi\hbar a}}\left(\frac{e^{-ipa/4\hbar} - e^{ipa/4\hbar}}{-ip/\hbar}\right)$$
$$= \frac{1}{2}\sqrt{\frac{a}{\pi\hbar}}Sinc\left(\frac{pa}{4\hbar}\right)$$

Thus, we have a continuum of momentum values from $-\infty < p < +\infty$ with the probability density

$$|\tilde{\varphi}(p)|^2 = \frac{a}{4\pi\hbar}Sinc^2\left(\frac{pa}{4\hbar}\right)$$

(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!

6.15.16 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 6.5 below).

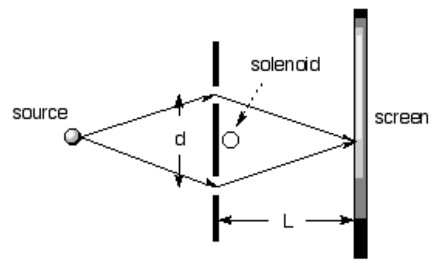


Figure 6.5: Aharonov-Bohm Setup

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

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

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

In the presence of a vector potential $\vec{A}$, minimal coupling says that

$$\vec{p} \to \vec{p} - \frac{e}{c}\vec{A}$$

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

$$\psi(\vec{r}, t) = \psi_1(\vec{r}, t)e^{\frac{i}{\hbar}\int^{\vec{r}} \frac{e}{c}\vec{A}\cdot d\vec{r}}$$

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,

$$\psi_1(\vec{r}, t) = \psi_0(\vec{r}, t) = \psi_0(\vec{r})e^{-iE_0 t/\hbar}$$

so that

$$\psi(\vec{r}, t) = \psi_0(\vec{r})e^{-iE_0 t/\hbar}e^{\frac{i}{\hbar}\int^{\vec{r}} \frac{e}{c}\vec{A}\cdot d\vec{r}}$$

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

When $I = 0$, for any point on the screen, the probability amplitude is

$$f = f_+ + f_-$$

where

$$\begin{aligned} f_+ &= \text{ amplitude from upper slit path} \\ f_- &= \text{ amplitude from lower slit path} \end{aligned}$$

When $I \neq 0$, we then have

$$f' = f'_+ + f'_-$$

where

$$\begin{aligned} f'_+ &= f_+ e^{\frac{i}{\hbar}\int_{C_+} \frac{e}{c}\vec{A}\cdot d\vec{r}} \\ f'_- &= f_- e^{\frac{i}{\hbar}\int_{C_-} \frac{e}{c}\vec{A}\cdot d\vec{r}} \end{aligned}$$

C_+ corresponds to the upper path and C_- corresponds to the lower path.

Therefore,

$$f' = f'_+ + f'_- = f_+ e^{\frac{i}{\hbar}\int\limits_{C_+} \frac{e}{c}\vec{A}\cdot d\vec{r}} + f_- e^{\frac{i}{\hbar}\int\limits_{C_-} \frac{e}{c}\vec{A}\cdot d\vec{r}} \propto f_+ + f_- e^{\frac{i}{\hbar}\left(\int\limits_{C_-} \frac{e}{c}\vec{A}\cdot d\vec{r} - \int\limits_{C_+} \frac{e}{c}\vec{A}\cdot d\vec{r}\right)}$$

or

$$f' \propto f_+ + f_- e^{\frac{i}{\hbar}\oint \frac{e}{c}\vec{A}\cdot d\vec{r}}$$

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 Δs, where assuming that $L \gg d$ and $L \gg \Delta s$, we find

$$\begin{aligned} \Delta s \tfrac{d}{L} k &= \tfrac{e\varphi}{\hbar c} = \text{ phase shift} \\ \Delta s &= \tfrac{e\varphi L}{\hbar c d k} = \tfrac{e\varphi L}{\hbar c d\sqrt{2mE_0}} \end{aligned}$$

6.15.17 A Josephson Junction

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

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

We consider a junction where

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

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

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

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

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

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 φ are given by

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

Using $\psi_i = \sqrt{n_i}e^{i\theta_i}$, we find

$$i\hbar\left(\tfrac{\dot{n}_1}{2\sqrt{n_1}}e^{i\theta_1} + i\dot{\theta}_1\sqrt{n_1}e^{i\theta_1}\right) = -\tfrac{ne^2}{C}\sqrt{n_1}e^{i\theta_1} - \tfrac{E_J}{n_0}\sqrt{n_2}e^{i\theta_2}$$
$$i\hbar\left(\tfrac{\dot{n}_2}{2\sqrt{n_2}}e^{i\theta_2} + i\dot{\theta}_2\sqrt{n_2}e^{i\theta_2}\right) = \tfrac{ne^2}{C}\sqrt{n_2}e^{i\theta_2} - \tfrac{E_J}{n_0}\sqrt{n_1}e^{i\theta_1}$$

or

$$i\hbar\tfrac{\dot{n}_1}{2} - \hbar n_1\dot{\theta}_1 = -\tfrac{ne^2}{C}n_1 - \tfrac{E_J}{n_0}\sqrt{n_1 n_2}e^{i\varphi}$$
$$i\hbar\tfrac{\dot{n}_2}{2} - \hbar n_2\dot{\theta}_2 = -\tfrac{ne^2}{C}n_2 - \tfrac{E_J}{n_0}\sqrt{n_1 n_2}e^{-i\varphi}$$

Taking real and imaginary parts,

$$\dot{\theta}_1 = \tfrac{ne^2}{\hbar C} + \tfrac{E_J}{\hbar n_0}\sqrt{\tfrac{n_2}{n_1}}\cos\varphi \quad , \quad \dot{\theta}_2 = -\tfrac{ne^2}{\hbar C} + \tfrac{E_J}{\hbar n_0}\sqrt{\tfrac{n_1}{n_2}}\cos\varphi$$
$$\dot{n}_1 = -\tfrac{E_J}{\hbar n_0}\sqrt{n_1 n_2}\sin\varphi \quad , \quad \dot{n}_2 = \tfrac{E_J}{\hbar n_0}\sqrt{n_1 n_2}\sin\varphi$$

Taking differences, we find the equations for n and φ,

$$\dot{\varphi} = \dot{\theta}_2 - \dot{\theta}_1 = -\tfrac{2ne^2}{\hbar C} - \tfrac{E_J}{\hbar n_0}\left(\sqrt{\tfrac{n_2}{n_1}} - \sqrt{\tfrac{n_1}{n_2}}\right)\cos\varphi \approx -\tfrac{2ne^2}{\hbar C}$$
$$\dot{n} = \dot{n}_2 - \dot{n}_1 = \tfrac{2E_J}{\hbar n_0}\sqrt{n_1 n_2}\sin\varphi \approx \tfrac{E_J}{\hbar}\sin\varphi$$

noting that $n_1 \approx n_2 \approx n_0/2$. Taking the sums, we find that $n =$ constant.

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

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

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

$$J_0 = \frac{eE_J}{\hbar} = \frac{2\pi e E_J}{h} = \frac{\pi E_J}{\phi_0}$$

(d) Show that

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

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

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

for small amplitudes.

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

We can exhibit oscillatory behavior as follows. We have

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

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

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

which gives $\varphi = \omega t$.

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

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

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

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

We have

$$\dot{\varphi} = -\frac{2ne^2}{\hbar C} = -\frac{2VCe}{\hbar C} = -\frac{2eV}{\hbar} = -\omega$$

which implies that $\varphi = -\omega t$

$$J_S = e\dot{n} = C\dot{V} = -C\frac{\hbar}{2e}\ddot{\varphi} = -C\frac{\hbar}{2e}\left(-\frac{2e^2 E_J}{\hbar^2 C}\sin\omega t\right) = J_0 \sin\omega t$$

where

$$J_0 = \frac{C\hbar}{2e}\frac{2e^2 E_J}{\hbar^2 C} = \frac{e E_J}{\hbar}$$

6.15.18 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

$$\hat{a} = \hat{b} + \alpha \quad , \quad \hat{a}^+ = \hat{b}^+ + \alpha^*$$

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

$$\hat{b}\,|0\rangle_b = 0 = (\hat{a} + \alpha)\,|0\rangle_b = 0 \to \hat{a}\,|0\rangle_b = \alpha\,|0\rangle_b = -V^*\,|0\rangle_b$$

The ground state is a coherent state.

6.15.19 Bogliubov Transformation

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

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

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

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

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

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

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

We have

$$\begin{aligned}\hat{b} &= \hat{a}\cosh\eta + \hat{a}^+\sinh\eta \\ \hat{b}^+ &= \hat{a}^+\cosh\eta + \hat{a}\sinh\eta\end{aligned}$$

Now using $[\hat{a}, \hat{a}^+] = 1$ we get

$$\begin{aligned}[\hat{b}, \hat{b}^+] &= [\hat{a}\cosh\eta + \hat{a}^+\sinh\eta, \hat{a}^+\cosh\eta + \hat{a}\sinh\eta] \\ &= \cosh^2\eta[\hat{a}, \hat{a}^+] - \sinh^2\eta[\hat{a}, \hat{a}^+] \\ &= \cosh^2\eta - \sinh^2\eta = 1\end{aligned}$$

so that the commutation relations are preserved.

We also have

$$\begin{aligned}\hat{a} &= \hat{b}\cosh\eta - \hat{b}^+\sinh\eta \\ \hat{a}^+ &= \hat{b}^+\cosh\eta - \hat{b}\sinh\eta\end{aligned}$$

Therefore,

$$\begin{aligned}\hat{H} &= \hbar\omega(\hat{b}^+\cosh\eta - \hat{b}\sinh\eta)(\hat{b}\cosh\eta - \hat{b}^+\sinh\eta) \\ &\quad + \frac{V}{2}((\hat{b}\cosh\eta - \hat{b}^+\sinh\eta)^2 + (\hat{b}^+\cosh\eta - \hat{b}\sinh\eta)^2) \\ &= \hbar\omega(\hat{b}^+\hat{b}\cosh^2\eta - (\hat{b}^+)^2\cosh\eta\sinh\eta - (\hat{b})^2\cosh\eta\sinh\eta + \hat{b}\hat{b}^+\sinh^2\eta) \\ &\quad + \frac{V}{2}(((\hat{b})^2)(\cosh^2\eta + \sinh^2\eta) + (\hat{b}^+)^2)(\cosh^2\eta + \sinh^2\eta) \\ &\quad - \hat{b}\hat{b}^+\cosh\eta\sinh\eta - \hat{b}^+\hat{b}\cosh\eta\sinh\eta)\end{aligned}$$

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

$$\sinh 2\eta = 2\cosh\eta\sinh\eta \quad , \quad \cosh^2\eta + \sinh^2\eta = 1$$

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

$$E_n = \Omega n + F \quad n = 0, 1, 2, ...$$

Now the coefficient of n must be > 0 to make physical sense (energy would go to $-\infty$). This says that

$$\Omega > 0 \to V < \hbar\omega\frac{1}{\tanh 2\eta} = \frac{(\hbar\omega)^2}{V}$$

which says that we must have

$$V < \hbar\omega$$

Finally, for $\hat{U} = e^{\left(\hat{a}\hat{a}+\hat{a}^+\hat{a}^+\right)\eta/2}$ and using

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

with $A = (\hat{a}\hat{a} + \hat{a}^+\hat{a}^+)\eta/2$ and using

$$[\hat{a}^+\hat{a}^+, \hat{a}] = -2\hat{a}^+ \quad , \quad [\hat{a}\hat{a}, \hat{a}^+] = 2\hat{a}$$

we have

$$\hat{U}\hat{a}\hat{U}^{-1} = \hat{a}\left(1 + \frac{\eta^2}{2!} + ...\right) - \hat{a}^+\hat{a}\left(\eta + \frac{\eta^3}{3!} + ...\right)$$

or

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

as before.

6.15.20 Harmonic oscillator

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

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

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

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

We first determine the position operator $x(t)$ in the Heisenberg representation. Using $[x, p] = i\hbar$ gives the operator equations of motion

$$\dot{x}(t) = \frac{i}{\hbar}[H, x] = \frac{i}{\hbar}\frac{1}{2m}(ppx - xpp) = \frac{i}{\hbar}\frac{1}{2m}(-2i\hbar p) = \frac{p(t)}{m}$$

$$\dot{p}(t) = \frac{i}{\hbar}[H, p] = \frac{i}{\hbar}\frac{m\omega^2}{2}(xxp - pxx) = \frac{i}{\hbar}\frac{m\omega^2}{2}(2i\hbar x) = -m\omega^2 x(t)$$

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 Schrodinger operators.

(b) Show that $e^{-\frac{i\hat{p}a}{\hbar}}$ 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

$$\begin{aligned}
\langle x\rangle &= \langle 0| e^{ipa/\hbar} x(t) e^{-ipa/\hbar} |0\rangle = \langle 0| \hat{I} e^{ipa/\hbar} x(t) e^{-ipa/\hbar} \hat{I} |0\rangle \\
&= \int dx' \int dx'' \langle 0 \,|\, x'\rangle \langle x'| e^{ipa/\hbar} x(t) e^{-ipa/\hbar} |x''\rangle \langle x'' \,|\, 0\rangle \\
&= \int dx' \int dx'' \langle 0 \,|\, x'\rangle \langle x' + a| \left(x\cos\omega t + \frac{p}{m\omega}\sin\omega t\right) |x'' + a\rangle \langle x'' \,|\, 0\rangle \\
&= \int dx' \int dx'' \langle 0 \,|\, x'\rangle \langle x' + a| ((x'' + a)\cos\omega t) |x'' + a\rangle \langle x'' \,|\, 0\rangle
\end{aligned}$$

where the p-term vanishes since

$$\langle 0| e^{ipa/\hbar} p e^{-ipa/\hbar} |0\rangle = \langle 0| p |0\rangle = 0$$

Now use

$$\int dx' \langle x'' + a \,|\, x'' + a \rangle = 1$$

to get

$$\langle x \rangle = \int dx \langle 0 \,|\, x \rangle (x + a) \cos \omega t \langle x \,|\, 0 \rangle = a \cos \omega t$$

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.

6.15.21 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

$$\begin{aligned}
\langle x(t) \rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle \psi| (a + a^+) |\psi\rangle \\
&= \frac{1}{3}\sqrt{\frac{\hbar}{2m\omega}} \left(e^{iE_0 t/\hbar} \langle 0| + e^{iE_1 t/\hbar} \langle 1| + e^{iE_2 t/\hbar} \langle 2| \right) (a + a^+) \left(e^{-iE_0 t/\hbar} |0\rangle + e^{-iE_1 t/\hbar} |1\rangle + e^{-iE_2 t/\hbar} |2\rangle \right) \\
&= \frac{1}{3}\sqrt{\frac{\hbar}{2m\omega}} \left(e^{i(E_0 - E_1)t/\hbar} \langle 0| \, a \, |1\rangle + e^{i(E_1 - E_2)t/\hbar} \langle 1| \, a \, |2\rangle + e^{i(E_1 - E_0)t/\hbar} \langle 1| \, a \, |0\rangle + e^{i(E_2 - E_1)t/\hbar} \langle 2| \, a \, |1\rangle \right) \\
&= \frac{1}{3}\sqrt{\frac{\hbar}{2m\omega}} \left(e^{-i\omega t} + e^{-i\omega t}\sqrt{2} + e^{i\omega t} + e^{i\omega t}\sqrt{2} \right) = \frac{1}{3}\sqrt{\frac{\hbar}{2m\omega}} (1 + \sqrt{2}) \cos \omega t
\end{aligned}$$

which oscillates with t.

6.15.22 The coherent state

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

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

where

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

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

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

$$\hat{a}|\alpha\rangle = \sum_{n=0}^{\infty} c_n \hat{a}|n\rangle = \sum_{n=0}^{\infty} c_n \hat{a}\sqrt{n}|n-1\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle$$

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

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

Thus, the coherent state is an eigenstate of the annihilation operator (α 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

$$\hat{x} = x_c \frac{\hat{a}+\hat{a}^+}{2} \quad x_c = \sqrt{\frac{2\hbar}{m\omega}}$$
$$\hat{p} = p_c \frac{\hat{a}-\hat{a}^+}{2i} \quad p_c = \sqrt{2m\hbar\omega}$$

Also

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \rightarrow \langle\alpha|\hat{a}^+ = \alpha^* \langle\alpha|$$

which implies that

$$\langle\alpha|\hat{a}|\alpha\rangle = \alpha\langle\alpha \mid \alpha\rangle = \alpha$$
$$\langle\alpha|\hat{a}^+|\alpha\rangle = \alpha^*\langle\alpha \mid \alpha\rangle = \alpha^*$$

and then

$$\langle\alpha|\,\hat{x}\,|\alpha\rangle = x_c\frac{\alpha+\alpha^*}{2} = x_c\mathrm{Re}(\alpha)$$
$$\langle\alpha|\,\hat{p}\,|\alpha\rangle = p_c\frac{\alpha-\alpha^*}{2i} = p_c\mathrm{Im}(\alpha)$$

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

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

$$\frac{d\psi}{\psi} = \frac{p_c}{\hbar}\left(\alpha-\frac{x}{x_c}\right)dx$$

which has the solution

$$\ln\frac{\psi}{\psi_0} = \frac{p_c}{\hbar}\left(\alpha x-\frac{x^2}{2x_c}\right)$$

or

$$\psi = \psi_0 e^{\frac{p_c}{\hbar}\left(\alpha x-\frac{x^2}{2x_c}\right)} = \psi_0 e^{ip_cIm(\alpha)x/\hbar}e^{\frac{p_c}{\hbar}\left(Re(\alpha)x-\frac{x^2}{2x_c}\right)}$$

if we let

$$Re(\alpha) = \frac{x_0}{x_c} \quad , \quad Im(\alpha) = \frac{p_0}{p_c}$$

we then have

$$\begin{aligned}\psi &= \psi_0 e^{ip_0x/\hbar}e^{\frac{p_c}{\hbar}\left(\frac{x_0x}{x_c}-\frac{x^2}{2x_c}\right)}\\ &= \psi_0 e^{ip_0x/\hbar}e^{\left(-\frac{p_c}{2\hbar x_c}x^2+\frac{x_0p_c}{\hbar x_c}x\right)}\\ &= \psi_0 e^{ip_0x/\hbar}e^{-\sqrt{\frac{p_c}{2\hbar x_c}}(x-x_0)^2}e^{-\frac{p_cx_0^2}{8\hbar x_c}}\\ &= \psi_0 e^{ip_0x/\hbar}u(x-x_0)\end{aligned}$$

where $\langle x\rangle = x_0$ and $\langle p\rangle = p_0$.

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

We have

$$\langle\hat{x}\rangle = x_0 = x_c\mathrm{Re}(\alpha) \to \mathrm{Re}(\alpha) = \frac{x_0}{x_c}$$

and

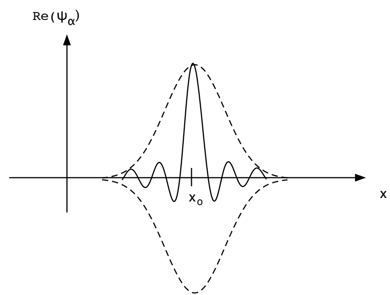
$$\langle\hat{p}\rangle = p_0 = p_c \text{Im}(\alpha) \to \text{Im}(\alpha) = \frac{p_0}{p_c}$$

so that

$$\alpha = \frac{x_0}{x_c} + i\frac{p_0}{p_c}$$

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

$$\tilde{\psi}_\alpha(p) = \mathcal{F}(e^{ip_0x/\hbar}) \circledast \mathcal{F}(u_0(x - x_0))$$

We have

$$\mathcal{F}(e^{ip_0x/\hbar}) = \delta(p - p_0)$$

and by the shift property

$$\mathcal{F}(u_0(x - x_0))e^{-ix_op/\hbar}\tilde{u}_0(p)$$

Therefore,

$$\tilde{\psi}_\alpha(p) = e^{-ix_op_0/\hbar}(e^{-ix_op/\hbar}\tilde{u}_0(p - p_0)$$

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

$$\Delta x^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 \quad , \quad \Delta p^2 = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$$

We already have $\langle \hat{x} \rangle = x_c Re(\alpha)$ and $\langle \hat{p} \rangle = p_c Im(\alpha)$. Now

$$\langle \hat{x}^2 \rangle = \frac{x_c^2}{4} \langle \alpha | (\hat{a}^2 + \hat{a}^{+\,2} + \hat{a}^+ \hat{a} + \hat{a}^+ \hat{a} \hat{a}^+) | \alpha \rangle$$

Using

$$\hat{a} | \alpha \rangle = \alpha | \alpha \rangle \rightarrow \langle \alpha | \hat{a}^+ = \alpha^* \langle \alpha |$$

we get

$$\begin{aligned} \langle \hat{x}^2 \rangle &= \frac{x_c^2}{4} \langle \alpha | (\alpha^2 + \alpha^{*\,2} + 2\alpha^* \alpha + \hat{a}^+ 1) | \alpha \rangle \\ &= \frac{x_c^2}{4} (\alpha + \alpha^*)^2 + \frac{x_c^2}{4} = (x_c Re(\alpha))^2 + \frac{x_c^2}{4} \\ &= \langle \hat{x} \rangle^2 + \frac{x_c^2}{4} \end{aligned}$$

or

$$(\Delta x)^2 = \frac{x_c^2}{4} \rightarrow \Delta x = \frac{x_c}{2} = \sqrt{\frac{\hbar}{2m\omega}}$$

and similarly

$$(\Delta p)^2 = \frac{p_c^2}{4} \rightarrow \Delta p = \frac{p_c}{2} = \sqrt{\frac{m\hbar\omega}{2}}$$

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,

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

Interpret this result.

At $t = 0$ we have $|\psi(0)\rangle = |\alpha\rangle$. Then

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t) |\psi(0)\rangle = \sum_{n=0}^{\infty} c_n \hat{U}(t) |n\rangle \\ &= \sum_{n=0}^{\infty} c_n e^{-iE_n t/\hbar} |n\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} c_n e^{-in\omega t} |n\rangle \end{aligned}$$

where

$$E_n = \hbar\omega(n+1/2) \quad , \quad c_n = e^{-|\alpha|^2/2}\frac{\alpha^n}{\sqrt{n!}}$$

We then have

$$\begin{aligned}|\psi(t)\rangle &= e^{-i\omega t/2}\sum_{n=0}^{\infty} e^{-|\alpha|^2/2}\frac{(\alpha e^{-in\omega t})^n}{\sqrt{n!}}|n\rangle \\ &= e^{-i\omega t/2}\sum_{n=0}^{\infty} e^{-|\alpha(t)|^2/2}\frac{(\alpha(t))^n}{\sqrt{n!}}|n\rangle\end{aligned}$$

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.

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

At later times

$$\langle\psi(t)|\,\hat{x}\,|\psi(t)\rangle = \langle\alpha(t)|\,\hat{x}\,|\alpha(t)\rangle = x_c Re(\alpha(t)) = x_c Re(\alpha e^{-i\omega t})$$

$$\langle\psi(t)|\,\hat{p}\,|\psi(t)\rangle = \langle\alpha(t)|\,\hat{p}\,|\alpha(t)\rangle = p_c Im(\alpha(t)) = x_c Im(\alpha e^{-i\omega t})$$

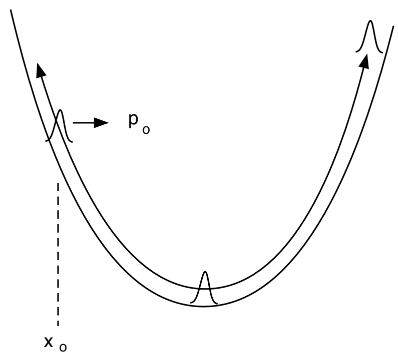
which are the classical equations of motion.

(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

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

$$\langle \hat{N} \rangle = \langle \alpha | \, \hat{a}^+ \hat{a} \, | \alpha \rangle = \alpha^* \alpha = |\alpha|^2$$

$$\Delta N = \sqrt{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2}$$

$$\begin{aligned} \sqrt{\langle \hat{N}^2 \rangle} &= \langle \alpha | \, (\hat{a}^+ \hat{a})^2 \, | \alpha \rangle = \langle \alpha | \, (\hat{a}^+ \hat{a})(\hat{a}^+ \hat{a}) \, | \alpha \rangle \\ &= \langle \alpha | \, (\hat{a}^{+\,2})(\hat{a})^2) \, | \alpha \rangle + \langle \alpha | \, \hat{a}^+ [\hat{a}, \hat{a}^+] \hat{a}) \, | \alpha \rangle \\ &= (\alpha^*)^2 (\alpha)^2 + (\alpha^*)(\alpha) = |\alpha|^4 + |\alpha|^2 \end{aligned}$$

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 uncertainly 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

$$P_n = | \, \langle n \, | \, \alpha \rangle \, |^2 = |c_n|^2 = |e^{-|\alpha|^2/2} \alpha^n / \sqrt{n!}|^2 = e^{-|\alpha|^2} \frac{(|\alpha|^2)^n}{\sqrt{n!}}$$

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!

6.15.23 Neutrino Oscillations

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

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

where

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

and

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

where we have used the basis

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

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

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

What is happening physically in this case?

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

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

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

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

We will do this problem in two equivalent ways, (1) differential equation method and (2) linear algebraic method.

We have

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \begin{pmatrix} M_0 & 0 & 0 \\ 0 & M_0 & 0 \\ 0 & 0 & M_0 \end{pmatrix} + \begin{pmatrix} 0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & 0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & 0 \end{pmatrix} = \begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix}$$

differential equation method: The Schrodinger equation is

$$\frac{\hbar}{i}\frac{\partial\psi}{\partial t} + \hat{H}\psi = 0$$

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

$$|\nu_1\rangle = |\nu_e\rangle \quad , \quad |\nu_2\rangle = |\nu_\mu\rangle \quad , \quad |\nu_3\rangle = |\nu_\tau\rangle$$

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

$$\begin{aligned} a_1(t) &= e^{-iM_0t/\hbar}a_1(0) \\ a_2(t) &= e^{-iM_0t/\hbar}a_2(0) \\ a_3(t) &= e^{-iM_0t/\hbar}a_3(0) \end{aligned}$$

or

$$\begin{pmatrix} a_1(t) \\ a_2(t) \\ a_3(t) \end{pmatrix} = \hat{U}(t) \begin{pmatrix} a_1(0) \\ a_2(0) \\ a_3(0) \end{pmatrix} = e^{-iM_0t/\hbar} \begin{pmatrix} a_1(0) \\ a_2(0) \\ a_3(0) \end{pmatrix}$$

If the neutrino is initially in one of the basis states, say, $|\nu_1\rangle$, then

$$\begin{pmatrix} a_1(0) \\ a_2(0) \\ a_3(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |\nu_1\rangle \rightarrow \begin{pmatrix} a_1(t) \\ a_2(t) \\ a_3(t) \end{pmatrix} = e^{-iM_0t/\hbar} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |\nu_1\rangle$$

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

$$\begin{aligned} i\hbar\dot{a}_1 &= M_0a_1 + \hbar\omega_1a_2 + \hbar\omega_1a_3 \\ i\hbar\dot{a}_2 &= M_0a_2 + \hbar\omega_1a_1 + \hbar\omega_1a_3 \\ i\hbar\dot{a}_3 &= M_0a_3 + \hbar\omega_1a_1 + \hbar\omega_1a_2 \end{aligned}$$

with boundary conditions

$$a_1(0) = 1 \quad , \quad a_2(0) = 0 \quad , \quad a_3(0) = 0$$

Let

$$\begin{aligned} a_1(t) &= e^{-iM_0t/\hbar}b_1(t) \rightarrow b_1(0) = 1 \\ a_2(t) &= e^{-iM_0t/\hbar}b_2(t) \rightarrow b_2(0) = 0 \\ a_3(t) &= e^{-iM_0t/\hbar}b_3(t) \rightarrow b_3(0) = 0 \end{aligned}$$

so that we get the new equations

$$\begin{aligned} \dot{b}_1 &= -i\omega_1(b_2 + b_3) \\ \dot{b}_2 &= -i\omega_1(b_1 + b_3) \\ \dot{b}_3 &= -i\omega_1(b_1 + b_2) \end{aligned}$$

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

$$\begin{aligned} \dot{b}_1 &= -2i\omega_1b_2 \\ \dot{b}_2 &= -i\omega_1b_2 - i\omega_1b_1 \end{aligned}$$

These give

$$\begin{aligned} &\ddot{b}_2 = -i\omega_1\dot{b}_2 - i\omega_1\dot{b}_1 = -i\omega_1\dot{b}_2 - 2\omega_1^2b_2 \\ &\ddot{b}_2 + i\omega_1\dot{b}_2 + 2\omega_1^2b_2 = 0 \end{aligned}$$

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 α.

$$-\alpha^2 + \omega_1\alpha + 2\omega_1^2 = 0 \to \alpha = -2\omega_1\ ,\ +\omega_1$$

Therefore, the most general solution is

$$b_2(t) = Ae^{i\omega_1 t} + Be^{-2i\omega_1 t}$$

Now,

$$b_2(0) = A + B = 0 \to B = -A$$

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

$$\dot{b}_1 = -2i\omega_1 b_2 = -2i\omega_1 A(e^{i\omega_1 t} - e^{-2i\omega_1 t})$$

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

$$b_1(0) = -3A = 1 \to A = -\frac{1}{3}$$

so that

$$b_1(t) = \tfrac{2}{3}\left(e^{i\omega_1 t} + \tfrac{1}{2}e^{-2i\omega_1 t}\right)$$
$$b_2(t) = -\tfrac{1}{3}(e^{i\omega_1 t} - e^{-2i\omega_1 t}) = b_3(t)$$

Finally,

$$\begin{aligned} P(\nu_e \to \nu_\mu; t) &= |a_2(t)|^2 = |b_2(t)|^2 = \left|-\frac{1}{3}(e^{i\omega_1 t} - e^{-2i\omega_1 t})\right|^2 \\ &= \frac{1}{9}\left|(e^{i\omega_1 t} - e^{-2i\omega_1 t})\right|^2 = \frac{1}{9}(2 - 2\cos 3\omega_1 t) = \frac{2}{9}(1 - \cos 3\omega_1 t) \\ &= P(\nu_e \to \nu_\tau; t) \end{aligned}$$

(c) The time of flight of the ν_e is $\Delta t = \ell/v$ in laboratory time. Therefore, the proper time is

$$\Delta\tau = \frac{\Delta t}{\gamma} = \Delta t\sqrt{1 - \frac{v^2}{c^2}} \approx \frac{\ell}{c}\frac{M_0}{E}$$

where $E =$ the total energy of the ν_e in the rest frame.

For $P(\nu_e \to \nu_\mu; t) \geq 0.01$ or

$$\frac{2}{9}(1 - \cos 3\omega_1\Delta\tau) \geq 0.01$$

we require that

$$\begin{aligned}
&1 - \cos 3\omega_1 \Delta\tau \geq 0.045 \\
&0.955 \geq \cos 3\omega_1 \Delta\tau \approx 1 - \tfrac{9}{2} \left(\omega_1 \Delta\tau\right)^2 \\
&\omega_1 \geq \tfrac{\sqrt{2}}{3} \sqrt{0.045} \tfrac{cE}{\ell M_0} \approx 0.1 \tfrac{cE}{\ell M_0} \\
&\hbar\omega_1 \geq 0.05\, eV
\end{aligned}$$

linear algebraic method: Let us find the eigenvalues and eigenvectors of $\hat{H}$.

The characteristic equation for the eigenvalues is

$$\begin{vmatrix} M_0 - E & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 - E & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 - E \end{vmatrix} = 0 = \left(M_0 - E\right)^3 - 3\left(M_0 - E\right)\left(\hbar\omega_1\right)^2 + 2\left(\hbar\omega_1\right)^3$$

or letting $\alpha = (M_0 - E)$ and $\beta = \hbar\omega_1$ we have the equation

$$\alpha^3 - 3\beta^2\alpha + 2\beta^3 = 0 \rightarrow \alpha = \beta,\ \beta,\ -2\beta$$

Therefore, the eigenvalues are

$$E_1 = M_0 + \hbar\omega_1\ ,\ E_2 = E_3 = M_0 - \hbar\omega_1\ (2 - \text{folddegeneracy})$$

Now we obtain the eigenvectors. For $E_1 = M_0 + \hbar\omega_1$ we have

$$\hat{H}\left|E_1\right\rangle = E_1\left|E_1\right\rangle = \left(M_0 + \hbar\omega_1\right)\left|E_1\right\rangle$$

or

$$\begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \left(M_0 + \hbar\omega_1\right) \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

or

$$\begin{aligned}
-2a + \ \ b + \ \ c &= 0 \\
a - 2b + \ \ c &= 0 \\
a + \ \ b - 2c &= 0
\end{aligned}$$

which imply that

$$a = b = c = \frac{1}{\sqrt{3}} (normalized\ to\ 1)$$

or

$$\left|E_1\right\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

In a similar manner, for $E_2 = E_3 = M_0 - \hbar\omega_1$ we have

$$\left|E_2\right\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \quad , \quad \left|E_3\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

Therefore,

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \sum_n |E_n\rangle \langle E_n \mid \psi(0)\rangle = \frac{1}{\sqrt{3}}|E_1\rangle + \frac{1}{\sqrt{6}}|E_2\rangle + \frac{1}{\sqrt{2}}|E_3\rangle$$

Using $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$, we have

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = \frac{1}{\sqrt{3}}e^{-iE_1t/\hbar}|E_1\rangle + \frac{1}{\sqrt{6}}e^{-iE_2t/\hbar}|E_2\rangle + \frac{1}{\sqrt{2}}e^{-iE_3t/\hbar}|E_3\rangle$$

Then,

$$P(\nu_e \to \nu_\tau; t) = |\langle \nu_\tau \mid \psi(t)\rangle|^2$$

where

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

or

$$\begin{aligned} P(\nu_e \to \nu_\tau; t) &= \left| \frac{1}{\sqrt{3}}e^{2i\omega_1 t}\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}}e^{-i\omega_1 t}\frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}}e^{-i\omega_1 t}\frac{1}{\sqrt{2}} \right|^2 \\ &= \frac{1}{9}\left| e^{3i\omega_1 t} - 1 \right|^2 = \frac{2}{9}(1 - \cos 3\omega_1 t) \end{aligned}$$

as above.

6.15.24 Generating Function

Use the generating function for Hermite polynomials

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

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

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

where

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

and

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

We have

$$\langle x \rangle_{nn'} = \int\limits_{-\infty}^{\infty} \psi_n^*(x) x \psi_{n'}(x) dx$$
$$= N_n N_{n'} \int\limits_{-\infty}^{\infty} dx\, H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2} x H_{n'}(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}$$
$$= \left(\frac{\alpha}{\sqrt{\pi} 2^n n!}\right)^{1/2} \left(\frac{\alpha}{\sqrt{\pi} 2^{n'} n'!}\right)^{1/2} \int\limits_{-\infty}^{\infty} dx\, e^{-\alpha^2 x^2} x H_n(\alpha x) H_{n'}(\alpha x)$$

Now

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

Therefore let $q = \alpha x$ and we have

$$\int_{-\infty}^{\infty} e^{-s^2+2sq} e^{-t^2+2tq} q e^{-q^2} dq = \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{s^n t^{n'}}{n! n'!} \int_{-\infty}^{\infty} H_n(q) H_{n'}(q) q e^{-q^2} dq$$

or

$$\sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{s^n t^{n'}}{n! n'!} A_{nn'} = \int_{-\infty}^{\infty} e^{-s^2+2sq} e^{-t^2+2tq} q e^{-q^2} dq$$

where

$$A_{nn'} = \int_{-\infty}^{\infty} H_n(\alpha x) H_{n'}(\alpha x) \alpha x e^{-\alpha^2 x^2} dx = \frac{1}{N_n} \frac{1}{N_{n'}} \langle x \rangle_{nn'}$$

Therefore, we are interested in the integral

$$\int_{-\infty}^{\infty} e^{-s^2+2sq} e^{-t^2+2tq} q e^{-q^2} dq = e^{-s^2-t^2} \int_{-\infty}^{\infty} e^{2(s+t)q} e^{-t^2+2tq} q e^{-q^2} dq$$
$$= e^{-s^2-t^2} \sqrt{\pi}(s+t) e^{(s+t)^2} = \sqrt{\pi}(s+t) e^{2st}$$

Finally we have

$$\sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{s^n t^{n'}}{n! n'!} A_{nn'} = \int_{-\infty}^{\infty} e^{-s^2+2sq} e^{-t^2+2tq} q e^{-q^2} dq$$
$$= e^{-s^2-t^2} \sqrt{\pi}(s+t) e^{(s+t)^2} = \sqrt{\pi}(s+t) e^{2st}$$

which allows us to determine $A_{nn'}$ term by term and thus determine $\langle x \rangle_{nn'}$

6.15.25 Given the wave function ......

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

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

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

(a) Find the mean position of the particle.

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx = \left(\frac{\gamma^2}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} x \exp\left(-\gamma^2 x^2\right) dx = 0$$

(b) Find the mean momentum of the particle.

$$\langle p\rangle = \int_{-\infty}^{\infty} \psi^*(x) \frac{\hbar}{i}\frac{d\psi(x)}{dx} \psi(x) dx = -\gamma^2 \frac{\hbar}{i} \left(\frac{\gamma^2}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} x \exp\left(-\gamma^2 x^2\right) dx = 0$$

(c) Find $V(x)$.

The Schrodinger equation gives

$$\begin{aligned}
&-\tfrac{\hbar^2}{2m}\tfrac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \to -\tfrac{\hbar^2}{2m}\tfrac{d^2\psi(x)}{dx^2} = (E - V(x))\psi(x) \\
&-\tfrac{\hbar^2}{2m}\left(-\gamma^2 + \gamma^4 x^2\right) e^{-\gamma^2 x^2/2} = (E - V(x)) e^{-\gamma^2 x^2/2} \\
&V(x) = E + \tfrac{\hbar^2}{2m}\left(-\gamma^2 + \gamma^4 x^2\right) = \tfrac{\hbar^2\gamma^4}{2m} x^2
\end{aligned}$$

(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

$$\psi(p) = N e^{-\frac{p^2}{2\hbar^2\gamma^2}} \quad , \quad N = \left(\frac{1}{\pi\hbar^2\gamma^2}\right)^{1/4}$$

which is an eigenfunction of the state with energy $E = \hbar^2\gamma^2/2m$ in the momentum representation.

Therefore,

$$P(p)dp = |\psi(p)|^2 dp = \left(\frac{1}{\pi\hbar^2\gamma^2}\right)^{1/2} e^{-\frac{p^2}{\hbar^2\gamma^2}} dp$$

Alternatively, $\psi(p)$ is the Fourier transform of $\psi(x)$, that is,

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-ipx/\hbar} \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-ipx/\hbar} \left(\frac{\gamma^2}{\pi}\right)^{1/4} \exp\left(-\gamma^2 x^2/2\right)$$
$$= \left(\frac{\gamma^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{p^2}{2\hbar^2\gamma^2}} \int \exp\left(\frac{p}{\sqrt{2}\hbar\gamma} - \frac{i\gamma x}{\sqrt{2}}\right)^2 dx = \left(\frac{1}{\pi\gamma^2\hbar^2}\right)^{1/4} e^{-\frac{p^2}{2\hbar^2\gamma^2}}$$

as above.

6.15.26 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

$$\langle x\rangle = \langle\alpha|\,\hat{x}\,|\alpha\rangle = \left(a^* \langle 0| + b^* \langle 1|\right) \hat{x} \left(a\,|0\rangle + b\,|1\rangle\right)$$

Now we have

$$\langle m|\,\hat{x}\,|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right)$$

Therefore,

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(a^* b + b^* a\right)$$

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

$$\frac{d\langle x\rangle}{da} = 0 \rightarrow a = b = \frac{1}{\sqrt{2}} \rightarrow \langle x\rangle_{\max} = \sqrt{\frac{\hbar}{2m\omega}}$$

and

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

(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:

$$\begin{aligned}\langle x(t)\rangle &= \langle\alpha(t)|\hat{x}|\alpha(t)\rangle \\ &= \frac{1}{2}\left(e^{i\omega t/2\hbar}\langle 0| + e^{i3\omega t/2\hbar}\langle 1|\right)\hat{x}\left(e^{-i\omega t/2\hbar}|0\rangle + e^{-i3\omega t/2\hbar}|1\rangle\right) \\ &= \frac{1}{2}\left(e^{-i\omega t/\hbar}\langle 0|\hat{x}|1\rangle + e^{i\omega t/\hbar}\langle 1|\hat{x}|0\rangle\right) \\ &= \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{2}\left(e^{-i\omega t/\hbar} + e^{i\omega t/\hbar}\right) = \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t\end{aligned}$$

Heisenberg Picture:

$$\begin{aligned}\langle x(t)\rangle &= \langle\alpha|\hat{x}(t)|\alpha\rangle = \langle\alpha|\hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t|\alpha\rangle \\ &= \frac{1}{2}\left(\cos\omega t\left(\langle 0|\hat{x}|1\rangle + \langle 1|\hat{x}|0\rangle\right) + \frac{1}{m\omega}\sin\omega t\left(\langle 0|\hat{p}|1\rangle + \langle 1|\hat{p}|0\rangle\right)\right) \\ &= \frac{1}{2}\left(\cos\omega t\left(\sqrt{\frac{\hbar}{2m\omega}} + \sqrt{\frac{\hbar}{2m\omega}}\right) + \frac{1}{m\omega}\sin\omega t\left(-\sqrt{\frac{\hbar m\omega}{2}} + \sqrt{\frac{\hbar m\omega}{2}}\right)\right) \\ &= \sqrt{\frac{\hbar}{2mw}}\cos\omega t\end{aligned}$$

which is the same for both pictures as expected.

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

Now using the Heisenberg picture we have

$$\left\langle(\Delta x)^2\right\rangle_t = \left\langle x^2\right\rangle_t - \langle x\rangle_t^2 = \langle\alpha|\hat{x}^2(t)|\alpha\rangle - \langle\alpha|\hat{x}(t)|\alpha\rangle^2$$

From (b) we have

$$\langle\alpha|\hat{x}(t)|\alpha\rangle = \sqrt{\frac{\hbar}{2mw}}\cos\omega t$$

The other term becomes

$$\begin{aligned}\langle\alpha|\hat{x}^2(t)|\alpha\rangle &= \frac{1}{2}\frac{\hbar}{2m\omega}\left(\langle 0| + \langle 1|\right)\left(e^{i\hat{H}t/\hbar}(\hat{a}+\hat{a}^+)^2 e^{-i\hat{H}t/\hbar}\right)\left(|0\rangle + |1\rangle\right) \\ &= \frac{1}{2}\frac{\hbar}{2m\omega}\left(\langle 0| + \langle 1|\right)\left(\hat{a}(t)\hat{a}(t) + \hat{a}(t)\hat{a}^+(t) + \hat{a}^+(t)\hat{a}(t) + \hat{a}^+(t)\hat{a}^+(t)\right)\left(|0\rangle + |1\rangle\right) \\ &= \frac{1}{2}\frac{\hbar}{2m\omega}\left(\langle 0| + \langle 1|\right)\left(\hat{a}\hat{a}e^{-2i\omega t} + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} + \hat{a}^+\hat{a}^+e^{2i\omega t}\right)\left(|0\rangle + |1\rangle\right) \\ &= \frac{1}{2}\frac{\hbar}{2m\omega}\left(\langle 1|\hat{a}\hat{a}^+|0\rangle + \langle 0|\hat{a}^+\hat{a}|1\rangle\right) = \frac{\hbar}{2m\omega}\end{aligned}$$

Therefore,

$$\left\langle(\Delta x)^2\right\rangle_t = \frac{\hbar}{2m\omega}\left(1 - \cos^2\omega t\right) = \frac{\hbar}{2m\omega}\sin^2\omega t$$

6.15.27 Coupled oscillators

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

We have

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{\rm int} = \frac{\hat{p}_1^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_2^2 + C\hat{x}_1\hat{x}_2$$

We shift to CM coordinates

$$\begin{array}{ll} \hat{X} = \hat{x}_1 - \hat{x}_2 \quad , & \hat{Y} = \frac{\hat{x}_1+\hat{x}_2}{2} \\ \hat{P} = \frac{\hat{p}_1-\hat{p}_2}{2} \quad , & \hat{\wp} = \hat{p}_1 + \hat{p}_2 \end{array}$$

or

$$\begin{array}{ll} \hat{x}_1 = \frac{\hat{X}}{2} + \hat{Y} \quad , & \hat{x}_2 = -\frac{\hat{X}}{2} + \hat{Y} \\ \hat{p}_1 = \hat{P} + \frac{\hat{\wp}}{2} \quad , & \hat{p}_2 = -\hat{P} + \frac{\hat{\wp}}{2} \end{array}$$

which gives

$$\hat{H} = \left[\frac{\hat{P}^2}{m} + \frac{mX^2}{4}\left(\omega^2 - \frac{C}{m}\right)\right] + \left[\frac{\hat{\wp}^2}{4m} + mY^2\left(\omega^2 + \frac{C}{m}\right)\right]$$

which represents two *uncoupled* oscillators.

The X-oscillator has frequency $\Omega_X = \sqrt{\omega^2 - C/m}$ and energy eigenvalues $E^X_{n_X} = \hbar\Omega_X(n_X + 1/2)$, $n_X = 0, 1, 2, ...$

The Y-oscillator has frequency $\Omega_Y = \sqrt{\omega^2 + C/m}$ and energy eigenvalues $E^Y_{n_Y} = \hbar\Omega_Y(n_Y + 1/2)$, $n_Y = 0, 1, 2, ...$

Therefore,

$$E_{n_X n_Y} = E^X_{n_X} + E^Y_{n_Y} = \hbar\Omega_X(n_X + 1/2) + \hbar\Omega_Y(n_Y + 1/2)$$

6.15.28 Interesting operators ....

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

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

(a) Show that

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

4. $\hat{c}^+ |0\rangle = |1\rangle \quad , \quad \hat{c} |0\rangle = 0$

We define

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

Then

$$\begin{aligned}
&\hat{N} = \hat{c}^+\hat{c} \to \hat{N}^+ = \left(\hat{c}^+\hat{c}\right)^+ = \hat{c}^+\hat{c} = \hat{N} \to Hermitian \\
&\hat{N}^2 = \hat{c}^+\hat{c}\hat{c}^+\hat{c} = \hat{c}^+\left(\hat{I} - \hat{c}^+\hat{c}\right)\hat{c} = \hat{c}^+\hat{c} = \hat{N}
\end{aligned}$$

Therefore,

$$\hat{N} |\lambda\rangle = \lambda |\lambda\rangle \to (\hat{N}^2 - \hat{N}) |\lambda\rangle = (\lambda^2 - \lambda) |\lambda\rangle = 0 \to \lambda = 0\,,\ 1$$

such that

$$\begin{aligned}
&\hat{N} |1\rangle = |1\rangle \to \hat{c}^+\hat{c} |1\rangle = |1\rangle \to \left(\hat{I} - \hat{c}\hat{c}^+\right) |1\rangle = |1\rangle \to \hat{c}\hat{c}^+ |1\rangle = 0 \\
&\hat{N} |0\rangle = 0 \to \hat{c}^+\hat{c} |0\rangle = 0 \to \left(\hat{I} - \hat{c}\hat{c}^+\right) |0\rangle = 0 \to \hat{c}\hat{c}^+ |0\rangle = |0\rangle
\end{aligned}$$

We then have

$$\begin{aligned}
&\langle 1| \hat{c}\hat{c}^+ |1\rangle = 0 = \left\|\hat{c}^+ |1\rangle\right\|^2 \to \hat{c}^+ |1\rangle = 0 \\
&\langle 0| \hat{c}^+\hat{c} |0\rangle = 0 = \left\|\hat{c} |0\rangle\right\|^2 \to \hat{c} |0\rangle = 0
\end{aligned}$$

Now

$$\langle 0| \hat{c}\hat{c}^+ |0\rangle = \langle 0 \mid 0\rangle = 1 \to \left\|\hat{c}^+ |0\rangle\right\|^2 = 1$$

If we suppose that

$$\begin{aligned}
&\hat{c}^+ |0\rangle = a |0\rangle + b |1\rangle \\
&\hat{c}^+\hat{c}^+ |0\rangle = 0 = a\hat{c}^+ |0\rangle + b\hat{c}^+ |1\rangle = a\hat{c}^+ |0\rangle
\end{aligned}$$

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

$$\langle 1| \hat{c}^+\hat{c} |1\rangle = \langle 1 \mid 1\rangle = 1 \to \left\|\hat{c} |1\rangle\right\|^2 = 1$$

If we suppose that

$$\begin{aligned}
&\hat{c} |1\rangle = a |1\rangle + b |0\rangle \\
&\hat{c}^+\hat{c} |1\rangle = 0 = a\hat{c} |1\rangle + b\hat{c} |0\rangle = a\hat{c} |1\rangle
\end{aligned}$$

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).

(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:

$$n = 0 \rightarrow a_0 = 1 \ , \ b_0 = 0 \rightarrow E_0 = \tfrac{\hbar\omega_0}{2}$$
$$n = 1 \rightarrow a_1 = 0 \ , \ b_1 = 1 \rightarrow E_1 = \tfrac{3\hbar\omega_0}{2}$$

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.

6.15.29 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

$$|\psi(0)\rangle = a\,|0\rangle + b\,|1\rangle$$
$$P(E = \hbar\omega/2) = |a|^2 = \tfrac{1}{2} \rightarrow a = \tfrac{1}{\sqrt{2}}$$
$$P(E = 3\hbar\omega/2) = |b|^2 = \tfrac{1}{2} \rightarrow b = \tfrac{1}{\sqrt{2}}e^{i\alpha}$$

so that

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i\alpha}\,|1\rangle\right)$$

Now

$$\begin{aligned}
\langle p\rangle_{t=0} &= \langle\psi(0)|\,\hat{p}\,|\psi(0)\rangle = \sqrt{\frac{m\omega\hbar}{2}} \\
&= \frac{i}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(\langle 0| + e^{-i\alpha}\langle 1|\right)\left(\hat{a}^{+} - \hat{a}\right)\left(|0\rangle + e^{i\alpha}|1\rangle\right) \\
&= \frac{i}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(-e^{i\alpha}\langle 0|\,\hat{a}\,|1\rangle + e^{-i\alpha}\langle 1|\,\hat{a}^{+}\,|0\rangle\right) \\
&= \frac{i}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(-e^{i\alpha} + e^{-i\alpha}\right) = \sin\alpha\sqrt{\frac{m\omega\hbar}{2}}
\end{aligned}$$

so that

$$\sin\alpha = 1 \to \alpha = \frac{\pi}{2}$$

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

$$\begin{aligned}
\langle p\rangle_{t} &= \langle\psi(t)|\,\hat{p}\,|\psi(t)\rangle \\
&= \frac{i}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(e^{i\omega t/2}\langle 0| - ie^{3i\omega t/2}\langle 1|\right)\left(\hat{a}^{+} - \hat{a}\right)\left(e^{-i\omega t/2}|0\rangle + ie^{-3i\omega t/2}|1\rangle\right) \\
&= \frac{i}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(-ie^{i\omega t}\langle 0|\,\hat{a}\,|1\rangle - ie^{-i\omega t}\langle 1|\,\hat{a}^{+}\,|0\rangle\right) \\
&= \frac{1}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(e^{-i\omega t} + e^{i\omega t}\right) = \sqrt{\frac{m\omega\hbar}{2}}\cos\omega t
\end{aligned}$$

6.15.30 Things about particles in box

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

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

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

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

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

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

We have

$$\psi(x,0) = \sum_n^{\infty} a_n \psi_n(x)$$

which gives

$$\int \psi_k^*(x)\psi(x,0)\,dx = \sum_n^{\infty} a_n \int \psi_k^*(x)\psi_n(x)\,dx = \sum_n^{\infty} a_n \delta_{nk} = a_k$$

Therefore

$$\begin{aligned} a_k &= \sqrt{60/\ell^6} \int_0^{\ell} x(\ell - x) \sin\frac{\pi k x}{\ell}\,dx \\ &= \sqrt{\frac{60}{\ell^6}} \frac{\ell^3}{k^3\pi^3} (2 - \cos k\pi + k\pi \sin k\pi) \\ &= \frac{8\sqrt{15}}{k^3\pi^3} \quad k = 1, 3, 5, ... \end{aligned}$$

and $a_k = 0$ for $k = 2, 4, ...$

Therefore,

$$\psi(x,0) = \sum_{m\ odd} \frac{8\sqrt{15}}{m^3\pi^3} \psi_m(x)$$

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

$$P(E_n) = |a_n|^2 = \begin{cases} \frac{960}{m^6\pi^6} & m = 1, 3, 5, ... \\ 0 & \text{otherwise} \end{cases}$$

NOTE: Since

$$\sum_n P(E_n) = 1$$

we have

$$\frac{960}{\pi^6} \sum_{n\ odd} \frac{1}{n^6} = 1 \rightarrow \sum_{n\ odd} \frac{1}{n^6} = \frac{\pi^6}{960} = 1.00145$$

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

$$\psi(x, t > 0) = \sum_{m\ odd} a_m \psi_m(x) e^{-iE_m t/\hbar}$$

6.15.31 Handling arbitrary barriers.....

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

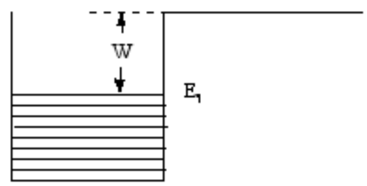


Figure 6.6: Finite Square Well

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

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

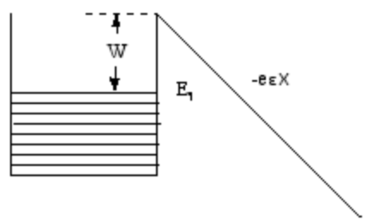


Figure 6.7: Finite Square Well + Electric Field

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

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

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

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

We have

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

where

$$(W+E_f)-e\varepsilon x = V(x) \quad \text{(assumes barrier maximum at x = 0)}$$

At $x = L$, we have

$$(W + E_f) - e\varepsilon L = E_f \to W = e\varepsilon L$$

Therefore,

$$T \approx \exp\left(-2\int_0^L \sqrt{\frac{2m}{\hbar^2}}\sqrt{(W + E_f) - e\varepsilon x - E_f dx}\right)$$
$$= \exp\left(-\sqrt{\frac{8m}{\hbar^2}}\int_0^L \sqrt{W - e\varepsilon x} dx\right)$$
$$= \exp\left(-\sqrt{\frac{8me\varepsilon}{\hbar^2}}\int_0^L \sqrt{L - x} dx\right) = \exp\left(-\frac{4}{3}\frac{\sqrt{2m}}{e\hbar}\frac{W^{3/2}}{\varepsilon}\right)$$

Approximating an Arbitrary Barrier

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

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

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

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

so that

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

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

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

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

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

Figure 6.8: Arbitrary Barrier Potential

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

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

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

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

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

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

6.15.32 Deuteron model

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

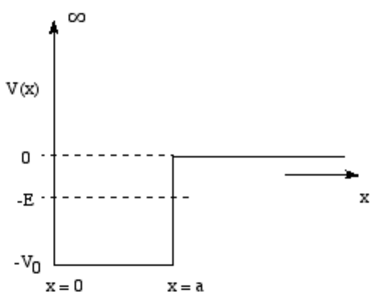


Figure 6.9: Deuteron Model

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

We have two regions to consider. We let $E = -|E|$. For $0 \le x \le a$

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad , \quad \frac{\hbar^2 k^2}{2m} = V_0 - |E|$$

For $x \ge a$

$$\psi_{II}(x) = Ce^{-\gamma x} \quad , \quad \frac{\hbar^2 \gamma^2}{2m} = |E|$$

We now impose boundary conditions at $x = 0$ and $x = a$:

$$\begin{array}{l} \psi_I(0) = 0 \to A = -B \to \psi_I(x) = A\sin kx \\ \psi_I(a) = \psi_{II}(a) \to A\sin ka = Ce^{-\gamma a} \\ \psi_I'(a) = \psi_{II}'(a) \to kA\cos ka = -\gamma Ce^{-\gamma a} \end{array}$$

These give

$$\tan ka = -\frac{k}{\gamma} \to \tan\left(\frac{2m\,|E|}{\hbar^2}a^2\right)^{1/2}\left(\frac{V_0}{|E|} - 1\right)^{1/2} = -\left(\frac{V_0}{|E|} - 1\right)^{1/2}$$

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

$$\left(\frac{V_0}{|E|} - 1\right)^{1/2} \approx 5.5 \to V_0 = 31.25\,|E| = 66.55\,MeV$$

6.15.33 Use Matrix Methods

A one-dimensional potential barrier is shown in the figure below.

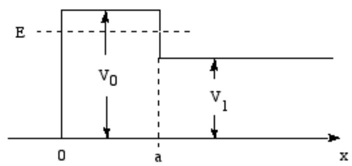


Figure 6.10: A Potential Barrier

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:

$$\text{(I)}\ \ x \leq 0 \quad , \quad E = \frac{\hbar^2 k^2}{2m} \quad \psi_I(x) = e^{ikx} + Re^{-ikx}$$

$$\text{(II)}\ \ 0 \leq x \leq a \quad , \quad V_0 - E = \frac{\hbar^2 \alpha^2}{2m} \quad \psi_{II}(x) = Ae^{-\alpha x} + Be^{\alpha x}$$

$$\text{(III)}\ \ x \geq a \quad , \quad E - V_1 = \frac{\hbar^2 k'^2}{2m} \quad \psi_{III}(x) = Te^{ikx}$$

Boundary conditions:

$$\begin{aligned}
&\psi_I(0) = \psi_{II}(0) \to 1 + R = A + B \\
&\psi_{II}(a) = \psi_{III}(a) \to Ae^{-\alpha a} + Be^{\alpha a} = Te^{ik'a} \\
&\frac{d}{dx}\psi_I(0) = \frac{d}{dx}\psi_{II}(0) \to ik(1 - R) = -\alpha(A - B) \\
&\frac{d}{dx}\psi_{II}(a) = \frac{d}{dx}\psi_{III}(a) \to -\alpha(Ae^{-\alpha a} - Be^{\alpha a}) = ik'Te^{ik'a}
\end{aligned}$$

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

$$\begin{pmatrix} 1 \\ R \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}^{-1}\begin{pmatrix} 1 & 1 \\ -\alpha & \alpha \end{pmatrix}\begin{pmatrix} e^{-\alpha a} & e^{\alpha a} \\ -\alpha e^{-\alpha a} & \alpha e^{\alpha a} \end{pmatrix}^{-1}\begin{pmatrix} 1 \\ ik' \end{pmatrix} Te^{ik'a} = M\begin{pmatrix} 1 \\ ik' \end{pmatrix} Te^{ik'a}$$

Therefore we have

$$M = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 \\ -\alpha & \alpha \end{pmatrix} \begin{pmatrix} e^{-\alpha a} & e^{\alpha a} \\ -\alpha e^{-\alpha a} & \alpha e^{\alpha a} \end{pmatrix}^{-1}$$
$$= \frac{1}{4i\alpha k} \begin{pmatrix} -ik & -1 \\ -ik & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -\alpha & \alpha \end{pmatrix} \begin{pmatrix} \alpha e^{\alpha a} & -e^{\alpha a} \\ \alpha e^{-\alpha a} & e^{-\alpha a} \end{pmatrix}$$
$$= \frac{1}{4i\alpha k} \begin{pmatrix} \alpha\left[(\alpha - ik) e^{\alpha a} - (\alpha + ik) e^{-\alpha a}\right] & \left[-(\alpha - ik) e^{\alpha a} - (\alpha + ik) e^{-\alpha a}\right] \\ \alpha\left[-(\alpha + ik) e^{\alpha a} + (\alpha - ik) e^{-\alpha a}\right] & \left[(\alpha + ik) e^{\alpha a} + (\alpha - ik) e^{-\alpha a}\right] \end{pmatrix}$$

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

$$T = \frac{-4i\alpha k e^{-ik'a}}{(\alpha - ik')(\alpha - ik) e^{\alpha a} - (\alpha + ik')(\alpha - ik) e^{-\alpha a}}$$
$$= \frac{-4i\alpha k e^{-ik'a}}{(\alpha^2 - kk') e^{\alpha a} - i\alpha(k + k')e^{\alpha a} - (\alpha^2 + kk') e^{-\alpha a} + i\alpha(k - k')e^{-\alpha a}}$$
$$= \frac{-4ie^{-ik'a}}{\left(\frac{\alpha}{k} - \frac{k'}{\alpha}\right) e^{\alpha a} - i\left(1 + \frac{k'}{k}\right) e^{\alpha a} - \left(\frac{\alpha}{k} + \frac{k'}{\alpha}\right) e^{-\alpha a} + i\left(1 - \frac{k'}{k}\right) e^{-\alpha a}}$$
$$= \frac{-2ie^{-ik'a}}{\left(\frac{\alpha}{k} - i\right)\sinh\alpha a - \left(i\frac{k'}{k} + \frac{k'}{\alpha}\right)\cosh\alpha a}$$

The limits $V_1 \to 0$, $k' \to k$, $a \to 2a$ give the standard result

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)}\sinh^2\alpha a}$$

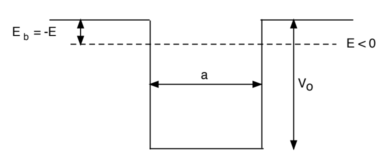
6.15.34 Finite Square Well Encore

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 $k_0 a/2$.

(i) $\frac{k_0 a}{2} = 1$, $(ii)\frac{k_0 a}{2} = 1.6$, $(iii)\frac{k_0 a}{2} = 5$

The finite square well is shown below



In Chapter 8 we showed that the solutions could be found as simultaneous solutions of:

Even Parity:

$$y = +x \tan x \quad , \quad x^2 + y^2 = r^2$$

Odd Parity:

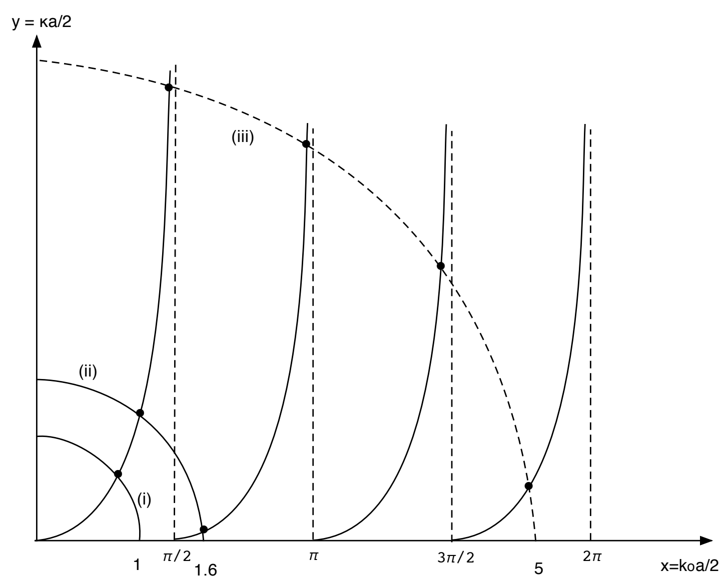
$$y = -x \cot x \quad , \quad x^2 + y^2 = r^2$$

where

$$y = \frac{\kappa a}{2} \quad , \quad x = \frac{ka}{2}$$

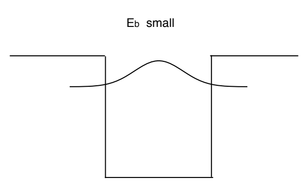
$$\kappa = \sqrt{\frac{2mE_b}{\hbar^2}} \quad , \quad k = \sqrt{\frac{2m(V_0 - E_b)}{\hbar^2}}$$

and $x, y > 0$, $r = k_0 a/2 > 0$. Shown below are the solutions for the three different choices of $r = k_0 a/2 > 0$.



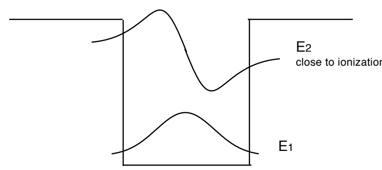
Case (i): $k_0 a/2 = 1$

We have one bound state with a wave function as shown below:



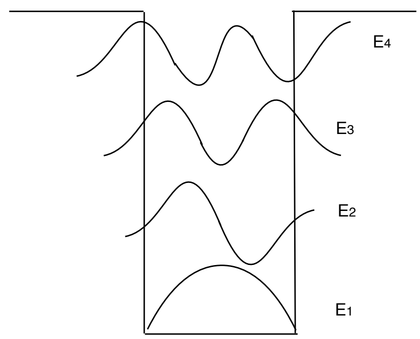
Case (ii): $k_0 a/2 = 1.6$

We have two bound states with a wave functions as shown below:



Case (iii): $k_0 a/2 = 5$

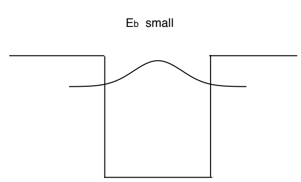
We have four bound states with a wave functions as shown below:



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 $0 < k_0 a/2 < \pi/2$. This is an even parity solution as shown below:



(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

$$\kappa a \to 0 \quad , \quad ka \to 0$$

and thus

$$\lim_{\kappa a, ka \to 0}\left(\frac{ka}{2}\tan\frac{ka}{2} = \frac{\kappa a}{2}\right) \to \frac{(ka)^2}{4} = \frac{\kappa a}{2}$$

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.

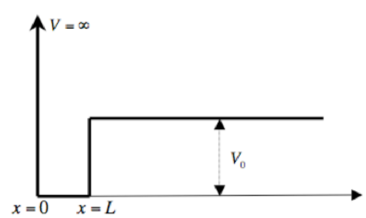


Figure 6.11: Half-Infinite, Half-Finite Well

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

$$\frac{k_0 a}{2} > \frac{\pi}{2} \to k_0 L > \frac{\pi}{2}$$

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

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

where

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

If we substitute

$$\frac{ka}{2} = kL$$

in the odd parity transcendental equation above we get

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

as required.

6.15.35 Half-Infinite Half-Finite Square Well Encore

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

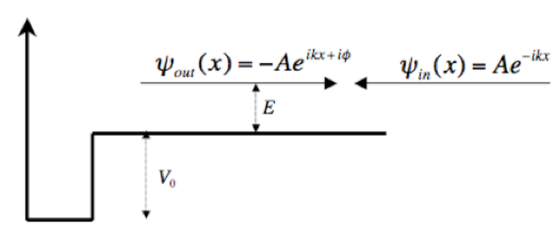
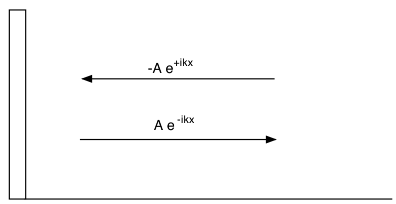


Figure 6.12: Half-Infinite, Half-Finite Well Again

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

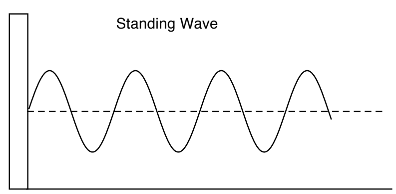
Warm Up: Consider a free particle on the half-line with an infinite wall at $x = 0$.



General solution to T.I.S.E.:

$$\psi(x) = Be^{ikx} + Ae^{-ikx} \quad , \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

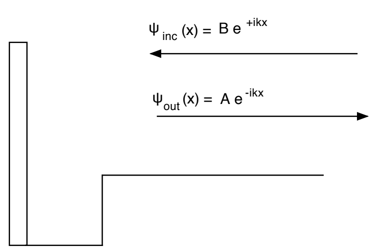
with boundary condition $\psi(0) = 0$, which implies that $B = -A$. This corresponds to a standing wave.



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 $x = +\infty$, $\psi_{inc} = Be^{ikx} = -Ae^{ikx}$ and the outgoing wave to $x = +\infty$, $\psi_{out} = -Aeikx$.

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

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

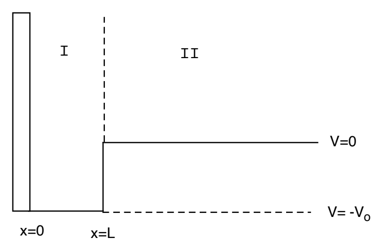
By conservation of probability

$$J_{inc} = J_{out} \to \frac{\hbar k}{m}|A|^2 = \frac{\hbar k}{m}|B|^2 \to |B| = |A|$$

We will look for solutions of the form

$$B = -Ae^{i\phi}$$

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:

$$u_I(x) = C\sin(qx) \quad , \quad q = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

Region II:

$$u_{II}(x) = Ae^{-ikx} + Be^{ikx} = Ae^{-ikx} - Ae^{ikx+i\phi} = -2iAe^{i\phi/2}\sin(kx+\phi/2)$$

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 ϕ as a function of $k_0 L$ for fixed energy. Comment on your plot.

When plotting ϕ, one should remember $\phi = \phi \, modulo \, 2\pi$ since ϕ and $\phi + 2\pi$ are the *same phase*.

We consider this as a function of $k_0 L$ for a fixed energy where

$$k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$$

Let

$$\bar{k} = \frac{k}{k_0} = \sqrt{\frac{E}{V_0}} \text{ take fixed}$$

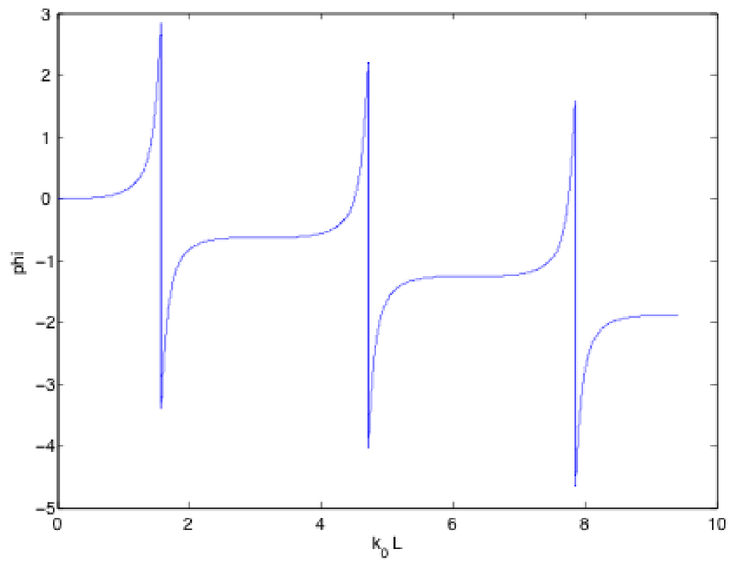
$$\frac{q}{k_0} = \left(\frac{E}{V_0} + 1\right)^{1/2} = (\bar{k}^2 + 1)^{1/2}$$

Let $\theta = k_0 L$. This then implies that

$$\phi = 2\tan^{-1}\left(\frac{\bar{k}}{\bar{k}^2 + 1)^{1/2}}\tan(\theta(\bar{k}^2 + 1)^{1/2}\right) - 2\bar{k}\theta$$

we want to plot this as a function of θ for a fixed $\bar{k}$ (i.e., change L). Shown below is a plot of $\phi(\theta)$ for $\bar{k} = \sqrt{E/V_0} = 0.1 \ll 1$ 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 θ except when $\theta = n\pi/2 = k_0L$. At these points the phase jumps by π.

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 π.

(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.

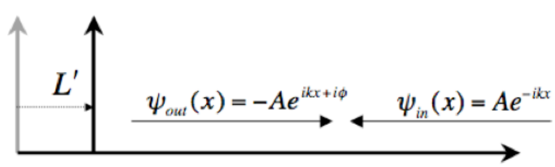


Figure 6.13: Shifted Wall

What is the effective L' as a function of the phase shift ϕ induced by our semi-finite well? What is the maximum value of L'? Can L' be negative? From your plot in (b), sketch L' as a function of k_0L, 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

6.15.36 Nuclear α 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.

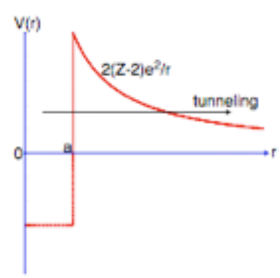


Figure 6.14: Nuclear Potential Model

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 α particle $1\,MeV$, $3\,MeV$, $10\,MeV$, $30\,MeV$.

We compute the integral

```
V = 2 (Z - 2) q^2 / r; tp = 2 (Z - 2) q^2 / E0;
Tint[r_] = Integrate[Sqrt[2 m (V - E0)], r]
```

$$\sqrt{2}\left(r\sqrt{m\left(-E0+\frac{2q^2(-2+Z)}{r}\right)} - \frac{2q^2\sqrt{r}\sqrt{m\left(-E0+\frac{2q^2(-2+Z)}{r}\right)}(-2+Z)\,\mathrm{Log}\left[2\sqrt{E0}\sqrt{r}+2\sqrt{4q^2+E0\,r-2q^2Z}\right]}{\sqrt{E0}\sqrt{4q^2+E0\,r-2q^2Z}}\right)$$

to give the turning points and probabilities

```
ergtomev = 624150.97;
constants = {m → 3727.37917 / (2.99792458 * 10^10)^2,
   ħ → 6.58211915 * 10^-22, Z → 92, a → 5 * 10^-13, q → 4.802 * 10^-10 * Sqrt[ergtomev]};
energies = {1, 3, 10, 30};
T = Exp[-2/ħ (Tint[b] - Tint[a])];
(tp /. E0 → energies /. constants) * .01
(T /. b → tp - $MachineEpsilon) /. E0 → energies /. constants // Re
```

```
{2.59064×10^-13, 8.63545×10^-14, 2.59064×10^-14, 8.63545×10^-15}
```

```
{4.08218×10^-128, 6.29166×10^-63, 3.4855×10^-23, 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 $b \to b - \epsilon$, where *epsilon* is the *MachineEpsilon*, or the upper bound of positive numbers δ for which $1.0 + \delta = 1.0$ on one's computer.

6.15.37 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.

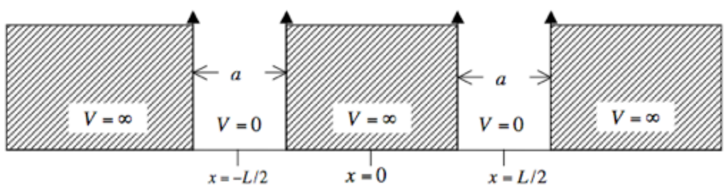


Figure 6.15: Two Boxes

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

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

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

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

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

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

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

$$P_{1+} = |\left\langle \phi_1^{(+)} \middle| \psi \right\rangle|^2 = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$$

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

The probability to find energy $\pi^2\hbar^2/2ma^2$ 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

$$P_{1+} = |\left\langle \phi_1^{(+)} \middle| \psi \right\rangle|^2 = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$$

$$P_{1-} = |\left\langle \phi_1^{(-)} \middle| \psi \right\rangle|^2 = \left(\frac{1}{2}\right)^2 = \frac{1}{4}$$

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

$$P_{left} = \sum_n |c_n^{(+)}|^2$$

The probability to be in the right well is

$$P_{right} = \sum_n |c_n^{(-)}|^2$$

where

$$\psi(x) = \sum_n c_n^{(+)}\phi_n^{(+)} + \sum_n c_n^{(-)}\phi_n^{(-)}$$

Thus, for our wave function

$$P_{left} = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$$

The probability to be in the right well is

$$P_{right} = \sum_n |c_n^{(-)}|^2 = \left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$$

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

$$P_{left}(t) = \sum_n \left| \left\langle \phi_n^{(+)} \,\middle|\, \psi(t) \right\rangle \right|^2 = \sum_n |c_n^{(+)}(t)|^2$$

where

$$|\psi(t)\rangle = \sum_n c_n^{(+)} e^{-iE_n t/\hbar} \left|\phi_n^{(+)}\right\rangle + \sum_n c_n^{(-)} e^{-iE_n t/\hbar} \left|\phi_n^{(-)}\right\rangle$$

NOTE: This expansion for $P_{left}(t)$ is only valid because $\left|\phi_n^{(+)}\right\rangle$ and $\left|\phi_n^{(-)}\right\rangle$ are orthogonal, since they do not overlap.

We then have

$$P_{left}(t) = \sum_n |c_n^{(+)}(t)|^2 = \sum_n |c_n^{(+)} e^{-iE_n t/\hbar}|^2 = \sum_n |c_n^{(+)}|^2$$

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.

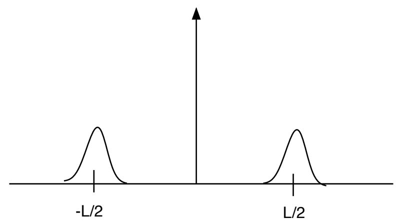
To show that this state is a stationary state we need to show that it is an eigenstate of $\hat{H}$.

$$\begin{aligned}
\hat{H}\Phi_n(x) &= \hat{H}(c_1\phi_n^{(+)}(x) + c_2\phi_n^{(-)}(x)) \\
&= c_1\hat{H}\phi_n^{(+)}(x) + c_2\hat{H}\phi_n^{(-)}(x) \\
&= c_1 E_n\phi_n^{(+)}(x) + c_2 E_n\phi_n^{(-)}(x) \\
&= E_n(c_1\phi_n^{(+)}(x) + c_2\phi_n^{(-)}(x)) = E_n\Phi_n(x)
\end{aligned}$$

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

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

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

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

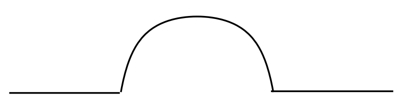
Therefore we can use shift-phase duality to write

$$\tilde{\phi}_n^{(\pm)}(p) = \tilde{u}_n(p)e^{\pm ipL/2\hbar}$$

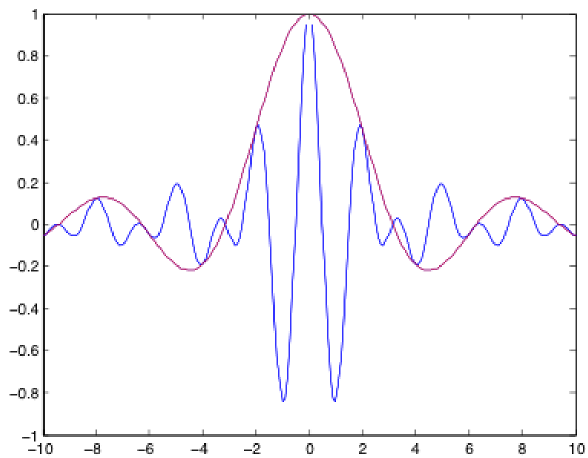
and thus

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

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 2π. The $x-$axis is $pL/2\hbar = pa/hbar$.

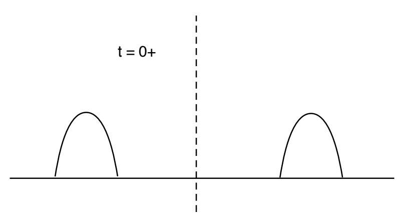
(i) Without calculation, what is the mean value $\langle p \rangle$? How does this change with time?

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.

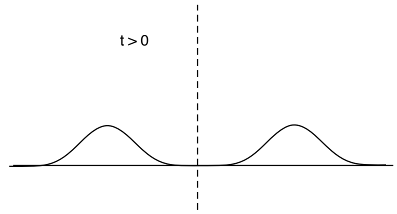
(j) Suppose the potential energy was somehow *turned off* (don't ask me how, just imagine it was done) so the particle is now free.

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.

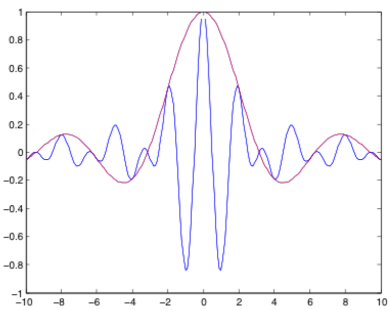
Suppose $V(x) \to 0$ instantaneously. This implies that the particle is now free. Right after the potential is turned off, $\psi(x)$ is the same state, say



Now the two wave packets spread



Eventually they overlap and interfere.



NOTE: this is just the two-slit problem.

6.15.38 A half-infinite/half-leaky box

Consider a one dimensional potential

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

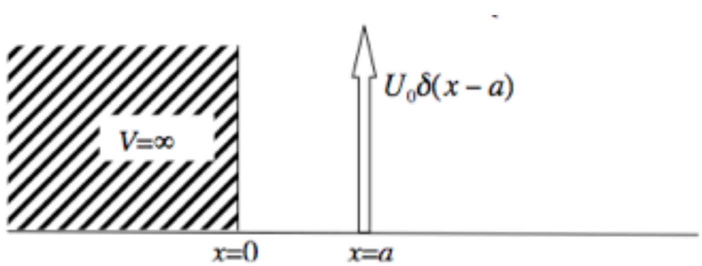


Figure 6.16: Infinite Wall + Delta Function

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

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

where

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

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

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

$$u(x) = A\sin(kx + \phi)$$

Region $0 < x < a$, boundary condition $u(0) = 0$, which implies that

$$u(x) = B\sin(kx)$$

where

$$E = \frac{\hbar^2 k^2}{2m} \to k = \sqrt{\frac{2mE}{\hbar^2}}$$

There are three unknowns, A, B, ϕ. We can eliminate two unknowns through the boundary conditions at $x = a$

$$u \text{ continuous } \to B\sin(ka) = A\sin(ka+\phi) \to B = A\frac{\sin(ka+\phi)}{\sin(ka)}$$

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 $\gamma_0 = 2mU_0/\hbar^2$. 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 ∞.

(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

$$u(x) = A\sin kx \quad x > 0$$

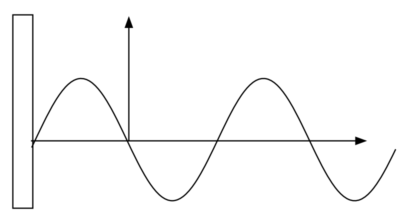
The limit $\gamma_0 \to \infty$ gives $\phi = -ka$, which implies that

$$u(x) = 0 \text{ inside} \qquad u(x) = A\sin(k(x-a)) \text{ outside}$$

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*.

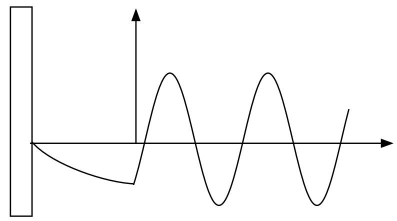
(d) Sketch the energy eigenfunction when $ka = \pi/2$. How does the probability to find the particle in the region $0 < x < a$ compare with that found in part (c)? Comment.

When $ka = \pi/2$,

$$\phi(k) = \tan^{-1}\left(\frac{k}{-\gamma_0}\right) - \frac{\pi}{2}$$

or

$$\frac{\sin(ka+\phi)}{\sin(ka)} = \sin\tan^{-1}\left(\frac{k}{-\gamma_0}\right) < 1$$



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.

(e) 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:

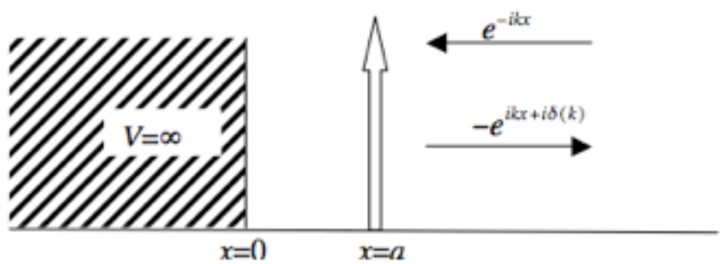


Figure 6.17: Scattering Scenario

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 $\rightarrow \infty$ here for the quasi-bound state. For this case, k is complex which implies finite lifetime!

6.15.39 Neutrino Oscillations Redux

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

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

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

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

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

Write down the eigenstates of m^2.

We construct the matrix

```
m2 = m02 {{1, 0}, {0, 1}} + dm2/2 {{-Cos[2 θ], Sin[2 θ]}, {Sin[2 θ], Cos[2 θ]}};
```

and solve for the eigenstates

```
Simplify[Eigensystem[m2], Assumptions → {dm2 > 0}]
{{-dm2/2 + m02, dm2/2 + m02}, {{-Cot[θ], 1}, {Tan[θ], 1}}}
```

We find the normalized eigenvalue/eigenvector pairs

$$\lambda_- = m_0^2 - \frac{\Delta m^2}{2} \quad , \quad |\nu-\rangle = \begin{pmatrix} -\cos\theta \\ \sin\theta \end{pmatrix}$$

$$\lambda_+ = m_0^2 + \frac{\Delta m^2}{2} \quad , \quad |\nu+\rangle = \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix}$$

(b) Calculate the probability for the state

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

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

The probability to measure

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

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

$$\begin{aligned}|\langle\psi(0)\,|\,\psi(t)\rangle\,|^2 &= |-\cos\theta\,\langle\psi(0)\,|\,\nu-\rangle\,e^{-iH_- t/\hbar} + \sin\theta\,\langle\psi(0)\,|\,\nu+\rangle\,e^{-iH_+ t/\hbar}|^2\\ &= |\cos^2\theta e^{-iH_- t/\hbar} + \sin^2\theta e^{-iH_+ t/\hbar}|^2\\ &= 1 - \sin^2(2\theta)\sin^2(H_+ - H_-)t/2\hbar\end{aligned}$$

Inserting the eigenvalues and recognizing that neutrinos are ultra-relativistic,

$$vert\,\langle\psi(0)\,|\,\psi(t)\rangle\,|^2 = 1 - \sin^2(2\theta)\sin^2\left(\frac{1}{4\hbar c}(\Delta m^2 c^4)\frac{t}{E}\right)$$

This can be massaged further to use experimentally convenient units:

$$\begin{aligned}|\langle\psi(0)\,|\,\psi(t)\rangle\,|^2 &= 1 - \sin^2(2\theta)\sin^2\left(\frac{GeV\,fm}{4\hbar c}(\frac{\Delta m^2 c^4}{eV^2})\frac{t}{E}\frac{GeV}{km}\right)\\ &= 1 - \sin^2(2\theta)\sin^2\left(1.267(\frac{\Delta m^2 c^4}{eV^2})\frac{t}{E}\frac{GeV}{km}\right)\end{aligned}$$

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

Let us implement the expression to try to recreate the baseline and periodicity (in units of km/MeV) in the data:

```
prob = 1 - s22t Sin[1.267 dm2c4 (1000 s)]^2;

Plot[prob /. {s22t → .8, dm2c4 → 8 * 10^-5}, {s, 0, 80}];
```

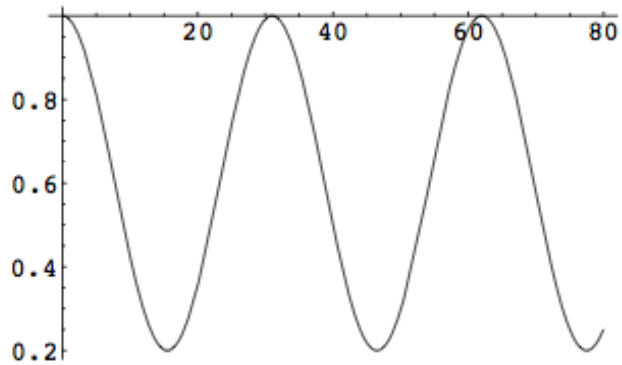


Figure 3 in the paper shows a peak-to-peak wavelength of a bit over $30\,km/MeV$, which is reproduced nicely here with the value of $\Delta m^2 = 8 \times 10^{-5}\,eV^2$ quoted in the paper. This is not surprising, as their quoted error is only $\pm 0.5 \times 10^{-5}\,eV^2$.

The amplitude and center of oscillation are more problematic, as this is entirely dependent on θ. 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 stong constraints on θ as shown in Figure 4(a). Looking at the 95% confidence range for just KamLAND, $0.1 < \tan^2\theta < 5$, or $0.33 < \sin^2\theta < 0.56$ passing through $\sin^2 = 1$. Examining Figure 3, the peak and through are at roughly 1.0 and 0.2 respectively, and this is reproduced above with the quoted value of $\sin^2\theta 0.8$ ($\tan^2\theta = 0.4$).

6.15.40 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

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

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

The wavefunction is

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

The probability for finding it in the ground state is given by

$$P = |\langle n=1 \,|\, \psi(x)\rangle|^2 = |\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\int_0^{a/2} \sin\left(\frac{\pi x}{a}\right) dx|^2$$

Thus,

$$P = |\frac{2}{a}\frac{a}{\pi}\int_0^{\pi/2} \sin q \, dq|^2 = \frac{4}{\pi^2} = 0.405$$

6.15.41 Some Thoughts on T-Violation

Any Hamiltonian can be recast to the form

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

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

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

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

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

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

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 the apparent T-violation due to complex phases. NOTE: This is the same problem as the neutrino oscillation (problem 8.39) if you set $E_i = \sqrt{p^2c^2 + m^2c^4} \approx pc + \frac{m^2c^3}{2p}$ and set all phases to zero.

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:

```
U2m = E^(I θ) ( Cos[θ] E^(I ϕ)    -Sin[θ] E^(I η) );
              ( Sin[θ] E^(-I η)   Cos[θ] E^(-I ϕ) )
E2m = ( E1  0  );
      ( 0   E2 )
amp212 = ( 0  1 ).U2m.MatrixExp[-I E2m t / ħ].Transpose[Conjugate[U2m]].( 1 );
                                                                        ( 0 )
p212 = ComplexExpand[Conjugate[amp212] * amp212];
amp221 = ( 1  0 ).U2m.MatrixExp[-I E2m t / ħ].Transpose[Conjugate[U2m]].( 0 );
                                                                        ( 1 )
p221 = ComplexExpand[Conjugate[amp221] * amp221];
TrigExpand[p212 - p221][[1, 1]]
```

```
0
```

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

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

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

Let us proceed in similar fashion as in the two-state problem above:

```
U3m = {{1, 0, 0}, {0, Cos[θ23], Sin[θ23]}, {0, -Sin[θ23], Cos[θ23]}}.
  {{Cos[θ13], 0, Sin[θ13] E^(-I δ)}, {0, 1, 0}, {-Sin[θ13] E^(I δ), 0, Cos[θ13]}}.{{Cos[θ12], Sin[θ12], 0}, {-Sin[θ12], Cos[θ12], 0}, {0, 0, 1}};
E3m = {{E1, 0, 0}, {0, E2, 0}, {0, 0, E3}};
amp312 = (0  1  0).U3m.MatrixExp[-I E3m t / ℏ].Transpose[Conjugate[U3m]].{{1}, {0}, {0}};
p312 = ComplexExpand[Conjugate[amp312] * amp312];
amp321 = (1  0  0).U3m.MatrixExp[-I E3m t / ℏ].Transpose[Conjugate[U3m]].{{0}, {1}, {0}};
p321 = ComplexExpand[Conjugate[amp321] * amp321];
Simplify[TrigExpand[p312 - p321]][[1, 1]]
```

$$-4 \cos[\theta 13]^2 \sin\left[\frac{(E1 - E2)\, t}{2 \hbar}\right] \sin\left[\frac{(E1 - E3)\, t}{2 \hbar}\right] \sin\left[\frac{(E2 - E3)\, t}{2 \hbar}\right] \sin[\delta] \sin[2\,\theta 12] \sin[\theta 13] \sin[2\,\theta 23]$$

Indeed, when $\delta \neq 0$, the two probabilities are different.

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

Again, as above, substituting $U \to U^*$:

```
amp3c12 = ( 0  1  0 ).Conjugate[U3m].MatrixExp[-I E3m t / ℏ].Transpose[U3m].(1, 0, 0);
p3c12 = ComplexExpand[Conjugate[amp3c12] * amp3c12];
amp3c21 = ( 1  0  0 ).Conjugate[U3m].MatrixExp[-I E3m t / ℏ].Transpose[U3m].(0, 1, 0);
p3c21 = ComplexExpand[Conjugate[amp3c21] * amp3c21];
```

$P(1 \to 2) - P(\bar{1} \to \bar{2})$:

```
Simplify[TrigExpand[p312 - p3c12]][[1, 1]]
```

$$-4\,\mathrm{Cos}[\theta 13]^2\,\mathrm{Sin}\left[\frac{(E1-E2)\,t}{2\hbar}\right]\mathrm{Sin}\left[\frac{(E1-E3)\,t}{2\hbar}\right]\mathrm{Sin}\left[\frac{(E2-E3)\,t}{2\hbar}\right]\mathrm{Sin}[\delta]\,\mathrm{Sin}[2\,\theta 12]\,\mathrm{Sin}[\theta 13]\,\mathrm{Sin}[2\,\theta 23]$$

$P(1 \to 2) - P(\bar{2} \to \bar{1})$:

```
TrigExpand[p312 - p3c21][[1, 1]]
```

```
0
```

6.15.42 Kronig-Penney Model

Consider a periodic repulsive potential of the form

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

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

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

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

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

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

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

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

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

Using the form of the wavefunction given in the problem,

$$\begin{aligned}
\psi(-\epsilon) &= A + B \\
\psi(+\epsilon) &= e^{ika}(Ae^{-ika} + Be^{ika}) \\
\psi'(-\epsilon) &= i\kappa(A + B) \\
\psi'(+\epsilon) &= i\kappa e^{ika}(Ae^{-ika} - Be^{ika})
\end{aligned}$$

which we now solve:

```
msol = Solve[{
  A + B == E^(I k a) (A E^(-I κ a) + B E^(I κ a)), I κ E^(I k a) (A E^(-I κ a) - B E^(I κ a)) - I κ (A - B) == (2 m λ)/ħ^2 (A + B)
 },
 {B, k}
];
```

Inserting the solution for k into the phase e^{ika}:

```
foo1 = FullSimplify[E^(I k a) /. msol, Assumptions → {ħ > 0, m > 0, λ > 0, κ > 0, a > 0}]
```

$$\left\{\frac{1}{2\hbar^2\kappa}\left(e^{-ia\kappa}\left(\hbar^2(1+e^{2ia\kappa})\kappa - i(-1+e^{2ia\kappa})m\lambda - 2\sqrt{e^{2ia\kappa}\left(-\hbar^4\kappa^2 + (\hbar^2\kappa\,\mathrm{Cos}[a\kappa] + m\lambda\,\mathrm{Sin}[a\kappa])^2\right)}\right)\right),\right.$$
$$\left.\frac{1}{2\hbar^2\kappa}\left(e^{-ia\kappa}\left(\hbar^2(1+e^{2ia\kappa})\kappa - i(-1+e^{2ia\kappa})m\lambda + 2\sqrt{e^{2ia\kappa}\left(-\hbar^4\kappa^2 + (\hbar^2\kappa\,\mathrm{Cos}[a\kappa] + m\lambda\,\mathrm{Sin}[a\kappa])^2\right)}\right)\right)\right\}$$

Making the suggested substitution $d = \hbar^2/m\lambda$:

```
phase = Expand[Simplify[foo1 /. λ → ℏ^2 / (m * d), Assumptions → {ℏ > 0, d > 0, κ > 0, a > 0}]]
```

$$\left\{\frac{1}{2} e^{-i a \kappa} + \frac{1}{2} e^{i a \kappa} + \frac{i e^{-i a \kappa}}{2 d \kappa} - \frac{i e^{i a \kappa}}{2 d \kappa} - \frac{e^{-i a \kappa} \sqrt{e^{2 i a \kappa} \left(d^2 \kappa^2 \text{Cos}[a \kappa]^2 + \text{Sin}[a \kappa]^2 + d \kappa (-d \kappa + \text{Sin}[2 a \kappa])\right)}}{d \kappa}, \frac{1}{2} e^{-i a \kappa} + \frac{1}{2} e^{i a \kappa} + \frac{i e^{-i a \kappa}}{2 d \kappa} - \frac{i e^{i a \kappa}}{2 d \kappa} + \frac{e^{-i a \kappa} \sqrt{e^{2 i a \kappa} \left(d^2 \kappa^2 \text{Cos}[a \kappa]^2 + \text{Sin}[a \kappa]^2 + d \kappa (-d \kappa + \text{Sin}[2 a \kappa])\right)}}{d \kappa}\right\}$$

We can read off the expressions for the two roots:

$$e^{ika} = \cos ka + \frac{1}{kd} \sin ka \pm \sqrt{\cos^2 ka + \frac{1}{(kd)^2} \sin^2 ka - 1 + \frac{1}{kd} \sin 2ka}$$

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

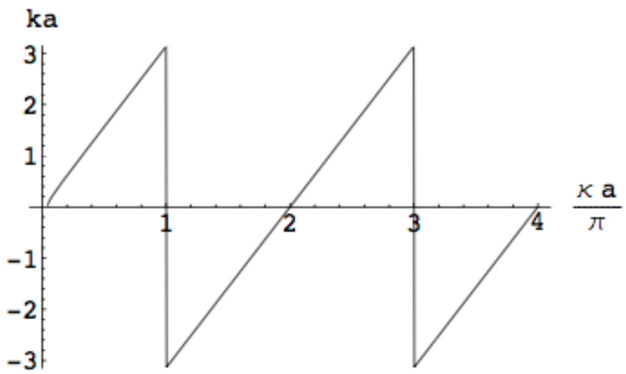
$$e^{ika} = \cos ka + \pm i \sqrt{1 - \cos^2 ka} = e^{\pm ika}$$

and so

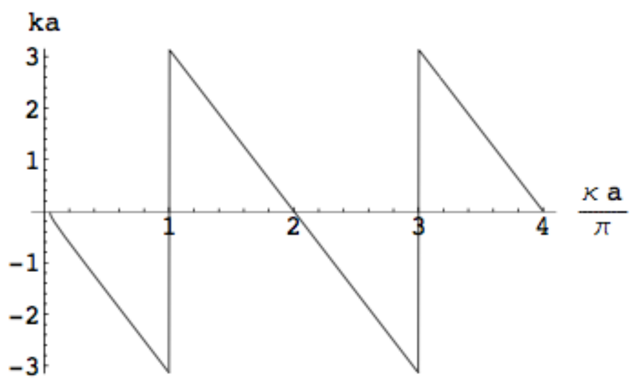
$$\kappa = \pm \left(k + \frac{2\pi n}{a}\right)$$

Equivalently, k is the momentum modulo $2\pi na$. Therefore, κ and hence the energy grow continuously as a function of k. This can be seen numerically with a d that is large enough:

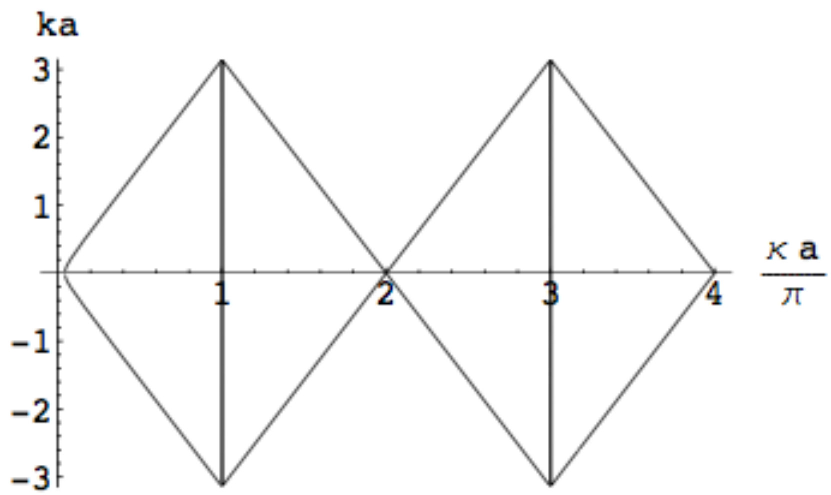
```
kplot1 = Plot[-I / a * Log[phase[[1]]] /. {a → 1, d → 100} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κa/π", "ka"}];
```




```
kplot2 = Plot[-I / a * Log[phase[[2]]] /. {a → 1, d → 100} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κa/π", "ka"}];
```



```
Show[kplot1, kplot2];
```



As we can see, no band gaps – every κ 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 ϵ,

$$\cos(n\pi + \epsilon) = (-1)^n \left(1 - \frac{\epsilon^2}{2} + O(\epsilon^4)\right)$$

$$\sin(n\pi + \epsilon) = (-1)^n \left(\epsilon + O(\epsilon^3)\right)$$

or

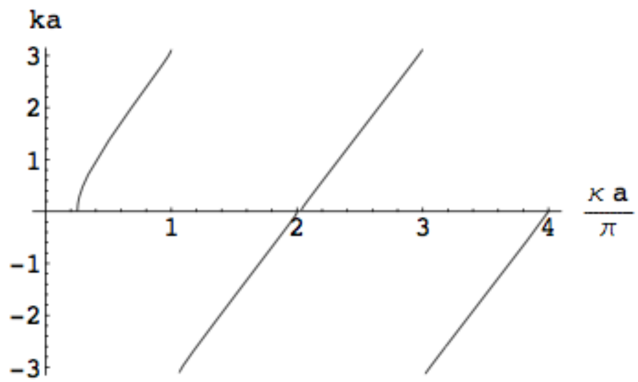
$$\cos ka + \frac{1}{kd}\sin ka = (-1)^n \left(1 + \frac{1}{kd}\epsilon - \frac{\epsilon^2}{2} + O(\epsilon^3)\right)$$

The magnitude exceeds 1 for $0 < \epsilon < 2/\kappa d \approx 2a/n\pi d$. 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 $\kappa = \pm\pi/a$.

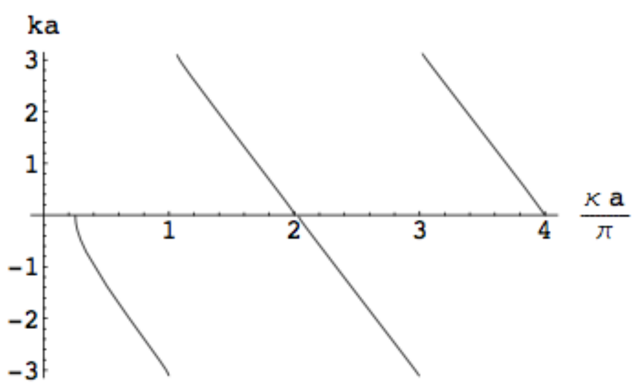
(d) Plot the relationship between κ and k for a weak potential ($d = 3a$) and a strong potential ($d = a/3$) (both solutions together).

Let us plot for the given cases as we did in (b), first the weak $d = 3a$:

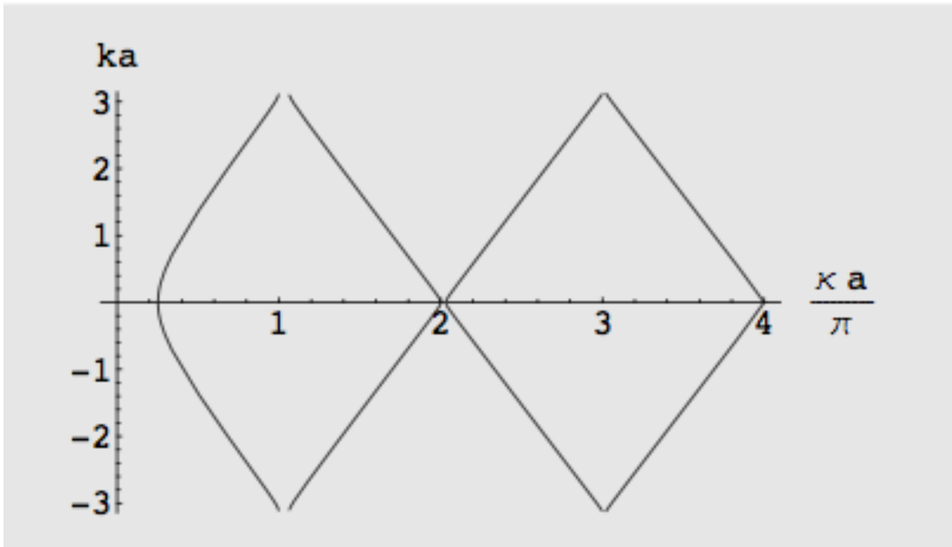
```
kplotcw1 = Plot[-I / a * Log[phase[[1]]] /. {a → 1, d → 3} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κ a / π", "ka"}];
```




```
kplotcw2 = Plot[-I / a * Log[phase[[2]]] /. {a → 1, d → 3} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κ a / π", "ka"}];
```



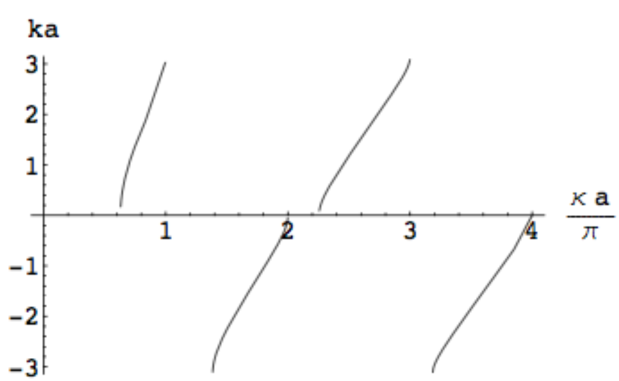
```
Show[kplotcw1, kplotcw2];
```



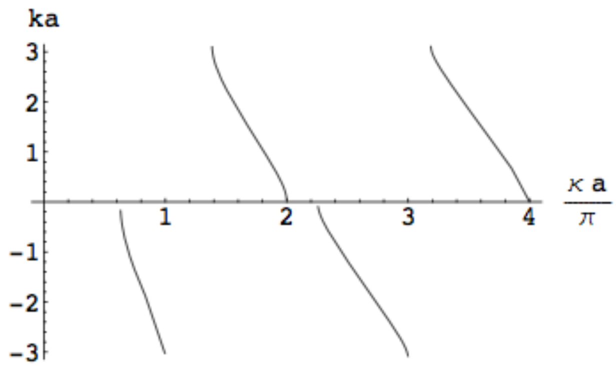
We see a big gap at $\kappa = 0$, a smaller one at $\kappa = \pi/a$, a yet smaller one at $\kappa = 2\pi/a$, and a gap you can barely see at $\kappa = 3\pi/a$. This is exactly what we predicted in part (c).

Now let us do the strong case $d = a/3$:

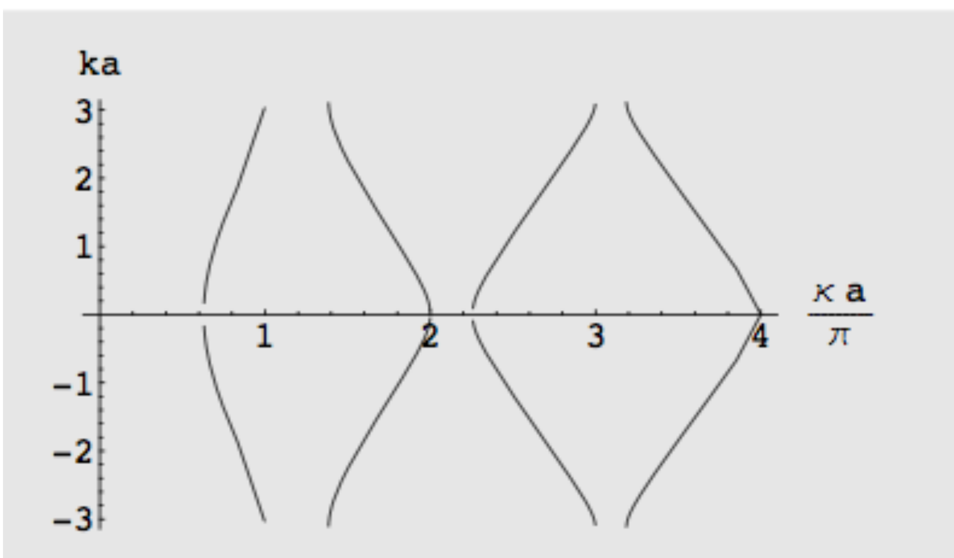
```
kplotcs1 = Plot[-I / a * Log[phase[[1]]] /. {a → 1, d → 1 / 3} /. κ → π * x,
  {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κ a / π", "ka"}];
```



```
kplotcs2 = Plot[-I / a * Log[phase[[2]]] /. {a → 1, d → 1 / 3} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κa/π", "ka"}];
```




```
Show[kplotcs1, kplotcs2];
```



Obviously, there is significant distortion from the free case in part (b), with gaps at $\kappa = n\pi/a$ much bigger than in the waeak case above.

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

It is the parity that changes the over all sign of k. This can be seen from the explicit form of the wave function,

$$\psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x} \quad \text{for } -a < x < 0$$

$$\psi(x) = e^{ika}(Ae^{i\kappa(x-a)} + Be^{-i\kappa(x-a)} \quad \text{for } 0 < x < a$$

The parity transformation gives

$$\begin{aligned}\psi(x) &= e^{ika}(Ae^{i\kappa(-x-a)} + Be^{-i\kappa(-x-a)} \\ &= Be^{i(k+\kappa)a}e^{i\kappa x} + Ae^{i(k-\kappa)a}e^{-i\kappa x} \\ &= A'e^{i\kappa x} + B'e^{-i\kappa x}\end{aligned}$$

and

$$\begin{aligned}\psi(x) &= Ae^{i\kappa x} + Be^{-i\kappa x} \\ &= e^{-ika}(Be^{i(k+\kappa)a}e^{i\kappa(x-a)} + Ae^{i(k-\kappa)a}e^{-i\kappa(x-a)}) \\ &= e^{-ika}(A'e^{i\kappa(x-a)} + B'e^{-i\kappa(x-a)})\end{aligned}$$

respectively. The two wave functions are related by the changes

$$A \to A' = Be^{i(k+\kappa)a}$$

$$B \to B' = Ae^{i(k-\kappa)a}$$

$$e^{ika} \to e^{-ika}$$

This is called Z_2 symmetry in k.

6.15.43 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,

$$e^{O_a} = I + O_a + \frac{1}{2!}O_a^2 + \frac{1}{3!}O_a^3 + ...$$

and insert the spectral decomposition

$$O_a = \sum_i \lambda_i P_i$$

This leads to

$$\begin{aligned} e^{O_a} &= I + \sum_i \lambda_i P_i + \frac{1}{2!}\sum_i \lambda_i^2 P_i + \frac{1}{3!}\sum_i \lambda_i^3 P_i + ... \\ &= \sum_i P_i + \sum_i \lambda_i P_i + \frac{1}{2!}\sum_i \lambda_i^2 P_i + \frac{1}{3!}\sum_i \lambda_i^3 P_i + ... \\ &= \sum_i \left(\sum_{n=0}^{\infty} \frac{\lambda_i^n}{n!}\right) P_i \\ &= \sum_i e^{\lambda_i} P_i \end{aligned}$$

(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 $\Delta)_a = 0$, it must be the case that $P_i |\Psi_a\rangle = |\Psi_a\rangle$ for some eigenspace projector. Then

$$E_a |\Psi_a\rangle = e^{\lambda_i} |\Psi_a\rangle$$

$$E_a^2 |\Psi_a\rangle = e^{2\lambda_i} |\Psi_a\rangle$$

$$\Delta E_a = 0$$

6.15.44 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

$$\langle O_x \rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$

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 b$\hbar$):

$$\frac{1}{\hbar} H = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \quad \lambda^2 - 1 = 0 \to \lambda = \pm 1$$

$$\lambda = +1 \to \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} \quad \lambda = -1 \to \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$\frac{1}{\hbar} H = \frac{1}{2} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix}$$

Thus,

$$\begin{aligned} e^{(-iHt/\hbar)} &= \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \left(\frac{1}{\hbar} H \right)^n \\ &= \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \frac{1}{2} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}^n \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \begin{pmatrix} e^{-it} & 0 \\ 0 & e^{it} \end{pmatrix} \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} e^{-it} + e^{it} & ie^{-it} - ie^{it} \\ -ie^{-it} + ie^{it} & e^{-it} + e^{it} \end{pmatrix} \\ &= \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix} \end{aligned}$$

so

$$|\Psi_a(t)\rangle = \begin{pmatrix} \cos(t) \\ -\sin(t) \end{pmatrix}$$

and at time t,

$$\begin{aligned}
\langle O_x \rangle &\to \begin{pmatrix} \cos(t) & -\sin(t) \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos(t) \\ -\sin(t) \end{pmatrix} \\
&= \begin{pmatrix} \cos(t) & -\sin(t) \end{pmatrix} \begin{pmatrix} -\sin(t) \\ \cos(t) \end{pmatrix} \\
&= -2\sin(t)\cos(t) = -\sin(2t)
\end{aligned}$$

$$\langle O_x^2 \rangle = 1$$

$$\Delta O_x = \sqrt{1 - \sin^2(2t)} = |\cos(2t)|$$

(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 ΔO_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

$$\begin{aligned}
\langle O_z \rangle &\to \begin{pmatrix} \cos(t) & -\sin(t) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos(t) \\ -\sin(t) \end{pmatrix} \\
&= \begin{pmatrix} \cos(t) & -\sin(t) \end{pmatrix} \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix} \\
&= \cos^2(t) - \sin^2(t) = \cos(2t)
\end{aligned}$$

$$\langle O_z^2 \rangle = 1$$

$$\Delta O_z = \sqrt{1 - \sin^2(2t)} = |\cos(2t)|$$

(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

$$\langle [O_x, O_z] \rangle = \begin{pmatrix} \cos(t) & -\sin(t) \end{pmatrix} \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} \begin{pmatrix} \cos(t) \\ -\sin(t) \end{pmatrix}$$

$$= \begin{pmatrix} \cos(t) & -\sin(t) \end{pmatrix} \begin{pmatrix} 2\sin(t) \\ 2\cos(t) \end{pmatrix}$$

$$= 0$$

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 ΔO_x or ΔO_z vanishes, i.e.,

$$t = \frac{n\pi}{4} \quad , \quad n = 0, 1, 2, ...$$

Chapter 7

Angular Momentum; 2- and 3-Dimensions

7.7 Problems

7.7.1 Position representation wave function

A system is found in the state

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

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

We have

$$\psi(\theta, \varphi) = \sqrt{\frac{15}{8\pi}} \cos\theta \sin\theta \cos\varphi = \sqrt{\frac{15}{8\pi}} \cos\theta \sin\theta \left(\frac{e^{i\varphi} + e^{-i\varphi}}{2}\right)$$

Now

$$Y_{2,\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{15}{8\pi}} \cos\theta \sin\theta e^{\pm i\varphi}$$

so that

$$\psi(\theta, \varphi) = \frac{1}{2}\left(-Y_{2,1}(\theta, \varphi) + Y_{2,-1}(\theta, \varphi)\right)$$

or

$$|\psi\rangle = \frac{1}{2}\left(-|2,1\rangle + |2,-1\rangle\right) \text{ using then notation } |L, L_z\rangle$$

The state is not normalized, that is,

$$\langle\psi \mid \psi\rangle = \frac{1}{4}(1+1) = \frac{1}{2}$$

so after proper normalization we have

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(-|2,1\rangle + |2,-1\rangle\right)$$

It is clear from the state vector that

$$L_z = \pm 1 \text{ each with probability } = 1/2$$

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

$$\begin{aligned}
\langle L_z \rangle &= \int\int \psi^* \hat{L}_z \psi \sin\theta d\theta d\varphi \\
&= \int\int \frac{1}{\sqrt{2}} \left(Y_{2,-1}^* - Y_{2,1}^*\right) \hat{L}_z \frac{1}{\sqrt{2}} \left(Y_{2,-1} - Y_{2,1}\right) d\Omega \\
&= \frac{\hbar}{2} \int\int \left(Y_{2,-1}^* - Y_{2,1}^*\right) \left(-Y_{2,-1} - Y_{2,1}\right) d\Omega \\
&= \frac{\hbar}{2} \left[-\int\int Y_{2,-1}^* Y_{2,-1}^* d\Omega + \int\int Y_{2,1}^* Y_{2,1} d\Omega \right] = \frac{\hbar}{2} [-1+1] = 0
\end{aligned}$$

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

$$\langle L_x \rangle = \frac{1}{\sqrt{2}} \left(-\langle 2,1| + \langle 2,-1|\right) \frac{\hat{L}_+ + \hat{L}_-}{2} \frac{1}{\sqrt{2}} \left(-|2,1\rangle + |2,-1\rangle\right) = \frac{1}{4}(0) = 0$$

since all the matrix elements are identically zero.

7.7.2 Operator identities

Show that

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

We have

$$\left[\vec{a}, \vec{b}\right] = \left[\vec{a}, \vec{L}\right] = \left[\vec{b}, \vec{L}\right] = 0$$

Using Einstein summation convention we have

$$\begin{aligned}
\left[\vec{a} \cdot \vec{L}, \vec{b} \cdot \vec{L}\right] &= (\vec{a} \cdot \vec{L})(\vec{b} \cdot \vec{L}) - (\vec{b} \cdot \vec{L})(\vec{a} \cdot \vec{L}) \\
&= (a_i L_i)(b_j L_j) - (b_j L_j)(a_i L_i) \\
&= a_i b_j [L_i, L_j] = a_i b_j i\hbar \varepsilon_{ijk} L_k \\
&= i\hbar \left(\vec{a} \times \vec{b}\right)_k L_k = i\hbar \left(\vec{a} \times \vec{b}\right) \cdot \vec{L}
\end{aligned}$$

(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

$$\begin{aligned}\left[\vec{L}^2,\vec{V}\right] &= \left[\left(\hat{L}_m\hat{L}_m\right),\left(\hat{V}_n\hat{e}_n\right)\right] = \left[\hat{L}_m\hat{L}_m,\hat{V}_n\right]\hat{e}_n = \hat{e}_n\left[\hat{L}_m\hat{L}_m\hat{V}_n - \hat{V}_n\hat{L}_m\hat{L}_m\right] \\ &= \hat{e}_n\left[\hat{L}_m\left(\left[\hat{L}_m,\hat{V}_n\right] + \hat{V}_n\hat{L}_m\right) - \left(\hat{L}_m\hat{V}_n - \left[\hat{L}_m,\hat{V}_n\right]\right)\hat{L}_m\right] \\ &= \hat{e}_n\left[\hat{L}_m\left[\hat{L}_m,\hat{V}_n\right] + \left[\hat{L}_m,\hat{V}_n\right]\hat{L}_m\right]\end{aligned}$$

Now for any vector operator we have

$$\left[\hat{L}_m,\hat{V}_n\right] = i\hbar\varepsilon_{mnp}\hat{V}_p$$

so that

$$\begin{aligned}\left[\vec{L}^2,\vec{V}\right] &= \hat{e}_n\left[\hat{L}_m\left[\hat{L}_m,\hat{V}_n\right] + \left[\hat{L}_m,\hat{V}_n\right]\hat{L}_m\right] \\ &= i\hbar\hat{e}_n\varepsilon_{mnp}\left[\hat{L}_m\hat{V}_p + \hat{V}_p\hat{L}_m\right] = i\hbar\left(\vec{V}\times\vec{L} - \vec{L}\times\vec{V}\right)\end{aligned}$$

Now consider

$$\left(\vec{L}\times\vec{V}\right)_1 = L_2V_3 - L_3V_2 = (V_3L_2 + i\hbar V_1) - (V_2L_3 - i\hbar V_1)$$

where we have used

$$\left[\hat{L}_m,\hat{V}_n\right] = i\hbar\varepsilon_{mnp}\hat{V}_p$$

Thus,

$$\left(\vec{L}\times\vec{V}\right)_1 = -\left(\vec{V}\times\vec{L}\right)_1 + 2i\hbar V_1$$

or

$$\vec{L}\times\vec{V} = \vec{V}\times\vec{L} + 2i\hbar\vec{V} \text{ for operators}$$

Therefore,

$$\left[\vec{L}^2,\vec{V}\right] = i\hbar\left(\vec{V}\times\vec{L} - \vec{L}\times\vec{V}\right) = 2i\hbar\left(\vec{V}\times\vec{L} - i\hbar\vec{V}\right)$$

7.7.3 More operator identities

Prove the identities

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

Using Einstein summation convention we have

$$\begin{aligned}\left(\vec{\sigma}\cdot\vec{A}\right)\left(\vec{\sigma}\cdot\vec{B}\right) &= A_iB_j\hat{\sigma}_i\hat{\sigma}_j = A_iB_j\left(\delta_{ij} + i\varepsilon_{ijk}\hat{\sigma}_k\right) \\ &= A_iB_j\delta_{ij} + i\varepsilon_{ijk}A_iB_j\hat{\sigma}_k = \vec{A}\cdot\vec{B} + i\vec{\sigma}\cdot\left(\vec{A}\times\vec{B}\right)\end{aligned}$$

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

Again using Einstein summation convention we have

$$e^{i\phi\vec{S}\cdot\hat{n}/\hbar}\vec{\sigma}e^{-i\phi\vec{S}\cdot\hat{n}/\hbar} = e^{i\phi\vec{\sigma}\cdot\hat{n}/2\hbar}\vec{\sigma}e^{-i\phi\vec{\sigma}\cdot\hat{n}/2\hbar}$$

and

$$e^{i\phi\vec{\sigma}\cdot\hat{n}/2\hbar} = \cos\frac{\phi}{2}\hat{I} + i\vec{\sigma}\cdot\hat{n}\sin\frac{\phi}{2}$$

Therefore,

$$\begin{aligned}
e^{i\phi\vec{S}\cdot\hat{n}/\hbar}\vec{\sigma}e^{-i\phi\vec{S}\cdot\hat{n}/\hbar} &= \left(\cos\frac{\phi}{2}\hat{I} + i\vec{\sigma}\cdot\hat{n}\sin\frac{\phi}{2}\right)\vec{\sigma}\left(\cos\frac{\phi}{2}\hat{I} - i\vec{\sigma}\cdot\hat{n}\sin\frac{\phi}{2}\right) \\
&= \cos^2\frac{\phi}{2}\vec{\sigma} + i\sin\frac{\phi}{2}\cos\frac{\phi}{2}\left[\vec{\sigma}\cdot\hat{n},\vec{\sigma}\right] + \sin^2\frac{\phi}{2}\left(\vec{\sigma}\cdot\hat{n}\right)\vec{\sigma}\left(\vec{\sigma}\cdot\hat{n}\right)
\end{aligned}$$

Now

$$\left[\vec{\sigma}\cdot\hat{n},\vec{\sigma}\right] = n_i\hat{e}_j\left[\sigma_i,\sigma_j\right] = 2in_i\hat{e}_j\varepsilon_{ijk}\sigma_k = 2i\varepsilon_{kij}\sigma_k n_i\hat{e}_j = 2i\left(\vec{\sigma}\times\hat{n}\right)$$

and

$$\begin{aligned}
\left(\vec{\sigma}\cdot\hat{n}\right)\vec{\sigma}\left(\vec{\sigma}\cdot\hat{n}\right) &= n_in_k\hat{e}_j\hat{\sigma}_i\hat{\sigma}_j\hat{\sigma}_k = n_in_k\hat{e}_j\hat{\sigma}_i\left(\delta_{jk} + i\varepsilon_{jkm}\hat{\sigma}_m\right) \\
&= n_in_k\hat{e}_j\hat{\sigma}_i\delta_{jk} + i\varepsilon_{jkm}n_in_k\hat{e}_j\hat{\sigma}_i\hat{\sigma}_m \\
&= n_in_j\hat{e}_j\hat{\sigma}_i + i\varepsilon_{jkm}n_in_k\hat{e}_j\left(\delta_{im} + i\varepsilon_{imp}\hat{\sigma}_p\right) \\
&= \hat{n}\left(\vec{\sigma}\cdot\hat{n}\right) + i\varepsilon_{jkm}n_in_k\hat{e}_j\delta_{im} - \varepsilon_{jkm}\varepsilon_{imp}n_in_k\hat{e}_j\hat{\sigma}_p \\
&= \hat{n}\left(\vec{\sigma}\cdot\hat{n}\right) + i\varepsilon_{jki}n_in_k\hat{e}_j + n_in_k\hat{e}_j\hat{\sigma}_p\varepsilon_{jkm}\varepsilon_{ipm} \\
&= \hat{n}\left(\vec{\sigma}\cdot\hat{n}\right) + i\left(\hat{n}\times\hat{n}\right) + n_in_k\hat{e}_j\hat{\sigma}_p\left(\delta_{ji}\delta_{kp} - \delta_{jp}\delta_{ki}\right) \\
&= \hat{n}\left(\vec{\sigma}\cdot\hat{n}\right) + n_in_j\hat{e}_i\hat{\sigma}_j - n_in_i\hat{e}_j\hat{\sigma}_j \\
&= \hat{n}\left(\vec{\sigma}\cdot\hat{n}\right) + \hat{n}\left(\vec{\sigma}\cdot\hat{n}\right) - \vec{\sigma}\left(\hat{n}\cdot\hat{n}\right) = 2\hat{n}\left(\vec{\sigma}\cdot\hat{n}\right) - \vec{\sigma}
\end{aligned}$$

Now

$$\hat{n}\times\left(\hat{n}\times\vec{\sigma}\right) = \left(\hat{n}\cdot\hat{n}\right)\vec{\sigma} - \left(\vec{\sigma}\cdot\hat{n}\right)\hat{n} \to \vec{\sigma} = \left(\vec{\sigma}\cdot\hat{n}\right)\hat{n} + \hat{n}\times\left(\hat{n}\times\vec{\sigma}\right)$$

so that

$$\left(\vec{\sigma}\cdot\hat{n}\right)\vec{\sigma}\left(\vec{\sigma}\cdot\hat{n}\right) = 2\hat{n}\left(\vec{\sigma}\cdot\hat{n}\right) - \vec{\sigma} = \left(\vec{\sigma}\cdot\hat{n}\right)\hat{n} - \hat{n}\times\left(\hat{n}\times\vec{\sigma}\right)$$

Finally,

$$\begin{aligned}
e^{i\phi\vec{S}\cdot\hat{n}/\hbar}\vec{\sigma}e^{-i\phi\vec{S}\cdot\hat{n}/\hbar} &= \cos^2\frac{\phi}{2}\vec{\sigma} + i\sin\frac{\phi}{2}\cos\frac{\phi}{2}\left[\vec{\sigma}\cdot\hat{n},\vec{\sigma}\right] + \sin^2\frac{\phi}{2}\left(\vec{\sigma}\cdot\hat{n}\right)\vec{\sigma}\left(\vec{\sigma}\cdot\hat{n}\right) \\
&= \cos^2\frac{\phi}{2}\left(\left(\vec{\sigma}\cdot\hat{n}\right)\hat{n} + \hat{n}\times\left(\hat{n}\times\vec{\sigma}\right)\right) - 2\sin\frac{\phi}{2}\cos\frac{\phi}{2}\left(\vec{\sigma}\times\hat{n}\right) \\
&\quad + \sin^2\frac{\phi}{2}\left(\left(\vec{\sigma}\cdot\hat{n}\right)\hat{n} - \hat{n}\times\left(\hat{n}\times\vec{\sigma}\right)\right) \\
&= \left(\vec{\sigma}\cdot\hat{n}\right)\hat{n} + \left(\hat{n}\times\left(\hat{n}\times\vec{\sigma}\right)\right)\cos\phi + \sin\phi\left(\hat{n}\times\vec{\sigma}\right)
\end{aligned}$$

7.7.4 On a circle

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

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

Solve the eigenvalue/eigenvector problem of H and interpret the degeneracy.

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

$$H = T + V = \frac{L_z^2}{2\mu a^2}$$

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

$$\begin{aligned}
&\left\langle\phi\right| H \left|\psi\right\rangle = \left\langle\phi\right| \tfrac{L_z^2}{2\mu a^2} \left|\psi\right\rangle = \left\langle\phi\right| E \left|\psi\right\rangle \\
&\tfrac{1}{2\mu a^2}\left(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\phi}\right)^2 \left\langle\phi \mid \psi\right\rangle = E\left\langle\phi \mid \psi\right\rangle \\
&-\tfrac{\hbar^2}{2\mu a^2}\tfrac{\partial^2\psi(\phi)}{\partial\phi^2} = E\psi(\phi)
\end{aligned}$$

so that we have the solution

$$\psi(\phi) = Ae^{im\phi} \quad , \quad E = \frac{\hbar^2 m^2}{2\mu a^2}$$

Now, imposing single-valuedness, we have

$$\begin{aligned}
&\psi(\phi) = Ae^{im\phi} = \psi(\phi + 2\pi) = Ae^{im\phi}e^{i2\pi m} \\
&e^{i2\pi m} = 1 \to m = \text{ integer}
\end{aligned}$$

Since m and $-m$ give the same energy, each level is 2-fold degenerate, corresponding to rotation CW and CCW.

7.7.5 Rigid rotator

A rigid rotator is immersed in a uniform magnetic field $\vec{B} = B_0\hat{e}_z$ so that the Hamiltonian is

$$\hat{H} = \frac{\hat{L}^2}{2I} + \omega_0\hat{L}_z$$

where ω_0 is a constant. If

$$\langle\theta, \phi \mid \psi(0)\rangle = \sqrt{\frac{3}{4\pi}}\sin\theta\sin\phi$$

what is $\langle \theta, \phi \mid \psi(t) \rangle$? What is $\left\langle \hat{L}_x \right\rangle$ at time t?

Preliminary work:

$$\begin{aligned} Y_{1,1} &= -\sqrt{\tfrac{3}{8\pi}} \sin\theta e^{i\varphi} = -\sqrt{\tfrac{3}{8\pi}} \tfrac{x+iy}{r} \\ Y_{1,-1} &= \sqrt{\tfrac{3}{8\pi}} \sin\theta e^{-i\varphi} = \sqrt{\tfrac{3}{8\pi}} \tfrac{x-iy}{r} \end{aligned}$$

Now

$$\langle \theta, \phi \mid \psi(0) \rangle = \sqrt{\frac{3}{4\pi}} \sin\theta \sin\phi = \sqrt{\frac{3}{4\pi}} \sin\theta \frac{e^{i\varphi} - e^{-i\varphi}}{2i} = \frac{i}{\sqrt{2}} Y_{1,1} + \frac{i}{\sqrt{2}} Y_{1,-1}$$

or

$$|\psi(0)\rangle = \frac{i}{\sqrt{2}} |1,1\rangle + \frac{i}{\sqrt{2}} |1,-1\rangle$$

Now,

$$\hat{H} = \frac{\hat{L}^2}{2I} + \omega_0 \hat{L}_z$$

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

$$\hat{H} |L,M\rangle = \frac{\hat{L}^2}{2I} |L,M\rangle + \omega_0 \hat{L}_z |L,M\rangle = \left(\frac{\hbar^2}{2I} L(L+1) + M\hbar\omega_0 \right) |L,M\rangle = E_{L.M} |L,M\rangle$$

Therefore,

$$|\psi(t)\rangle = \frac{i}{\sqrt{2}} e^{-iE_{1,1}t/\hbar} |1,1\rangle + \frac{i}{\sqrt{2}} e^{-iE_{1,-1}t/\hbar} |1,-1\rangle = \frac{i}{\sqrt{2}} e^{-i\frac{\hbar}{I}t} \left(e^{-i\omega_0 t} |1,1\rangle + e^{i\omega_0 t} |1,-1\rangle \right)$$

so that

$$\begin{aligned} \langle \theta, \phi \mid \psi(t) \rangle &= \frac{i}{\sqrt{2}} e^{-i\frac{\hbar}{I}t} \left(e^{-i\omega_0 t} Y_{1,1} + e^{i\omega_0 t} Y_{1,-1} \right) \\ &= \frac{i}{\sqrt{2}} e^{-i\frac{\hbar}{I}t} \sqrt{\frac{3}{8\pi}} \sin\theta \left(e^{-i\omega_0 t} e^{i\varphi} + e^{i\omega_0 t} e^{-i\varphi} \right) \\ &= e^{-i\frac{\hbar}{I}t} \sqrt{\frac{3}{4\pi}} \sin\theta \sin(\varphi - \omega_0 t) \end{aligned}$$

Finally,

$$\left\langle \hat{L}_x \right\rangle_t = \langle \psi(t) | \hat{L}_x | \psi(t) \rangle = \frac{1}{2} \langle \psi(t) | (\hat{L}_+ + \hat{L}_-) | \psi(t) \rangle = 0$$

since states making up $|\psi(t)\rangle$ have $\Delta M = 0, \pm 2$ only.

7.7.6 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

$$\begin{aligned}\psi(\rho,\phi) &= Ae^{-\rho^2/2\Delta}\cos^2\phi = Ae^{-\rho^2/2\Delta}\left(\frac{e^{i\phi}+e^{-i\phi}}{2}\right)^2 \\ &= \frac{A}{4}e^{-\rho^2/2\Delta}\left(2+e^{2i\phi}+e^{-2i\phi}\right)\end{aligned}$$

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

$$\begin{aligned}P(L_z = 0|\psi) &= |\langle L_z = 0 \mid \psi\rangle|^2 = \tfrac{2}{3} \\ P(L_z = +2|\psi) &= |\langle L_z = +2 \mid \psi\rangle|^2 = \tfrac{1}{6} \\ P(L_z = -2|\psi) &= |\langle L_z = -2 \mid \psi\rangle|^2 = \tfrac{1}{6}\end{aligned}$$

7.7.7 $L = 1$ System

Consider the following operators on a 3-dimensional Hilbert space

$$L_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \;,\; L_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \;,\; L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(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, $L_z \pm 1\,,\, 0$. The corresponding eigenvectors are

$$|L_z = +1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |1\rangle \quad , \quad |L_z = -1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = |-1\rangle \quad , \quad |L_z = 0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = |0\rangle$$

(b) Take the state in which $L_z = 1$. In this state, what are $\langle L_x\rangle$, $\left\langle L_x^2\right\rangle$ and $\Delta L_x = \sqrt{\langle L_x^2\rangle - \langle L_x\rangle^2}$.

We have

$$\langle L_x \rangle = \langle 1| L_x |1\rangle = (1,0,0)\,\tfrac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = 0$$

$$\langle L_x^2 \rangle = \langle 1| L_x^2 |1\rangle = (1,0,0)\,\tfrac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \tfrac{1}{2}$$

$$\Delta L_x = \sqrt{\langle L_x^2 \rangle - \langle L_x \rangle^2} = \sqrt{1/2} = 0.707$$

(c) Find the normalized eigenstates and eigenvalues of L_x in the L_z basis.

We use

$$\det |L_x - \lambda I| = 0 = -\lambda^3 + \lambda \to \lambda = \pm 1, 0$$

or we get the same eigenvalues as for L_z as expected. To fin d 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

$$|L_x = -1\rangle = \begin{pmatrix} 1/2 \\ -1/\sqrt{2} \\ 1/2 \end{pmatrix} = \tfrac{1}{2} |L_z = 1\rangle - \tfrac{1}{\sqrt{2}} |L_z = 0\rangle + \tfrac{1}{2} |L_z = -1\rangle$$

$$|L_x = 0\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix} = \tfrac{1}{\sqrt{2}} |L_z = 1\rangle - \tfrac{1}{\sqrt{2}} |L_z = -1\rangle$$

(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

$$\begin{aligned}
P(L_x = 1|L_z = -1) &= |\langle L_x = 1 \mid L_z = -1\rangle|^2 = \tfrac{1}{4} \\
P(L_x = 0|L_z = -1) &= |\langle L_x = 0 \mid L_z = -1\rangle|^2 = \tfrac{1}{2} \\
P(L_x = -1|L_z = -1) &= |\langle L_x = -1 \mid L_z = -1\rangle|^2 = \tfrac{1}{4}
\end{aligned}$$

(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

$$\begin{aligned}
L_z^2 |L_z = 1\rangle &= |L_z = 1\rangle \rightarrow \text{ eigenvalue } = +1 \\
L_z^2 |L_z = 0\rangle &= 0 \rightarrow \text{ eigenvalue } = 0 \\
L_z^2 |L_z = -1\rangle &= |L_z = -1\rangle \rightarrow \text{ eigenvalue } = +1
\end{aligned}$$

and

$$\begin{aligned}
P(L_z = 1|\psi) &= |\langle L_z = 1 \mid \psi\rangle|^2 = \tfrac{1}{4} \\
P(L_z = 0|\psi) &= |\langle L_z = 0 \mid \psi\rangle|^2 = \tfrac{1}{4} \\
P(L_z = -1|\psi) &= |\langle L_z = -1 \mid \psi\rangle|^2 = \tfrac{1}{2}
\end{aligned}$$

so written in the L_z^2 basis states labeled by $\left|L_z^2, L_z\right\rangle$ 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

$$|\psi_{new}\rangle = \sqrt{\frac{1}{3}} |1, 1\rangle + \sqrt{\frac{2}{3}} |1, -1\rangle$$

so that

$$L_z^2 |\psi_{new}\rangle = |\psi_{new}\rangle \rightarrow \text{ eigenvalue } = +1$$

and

$$\begin{aligned}
P(L_z^2 = 1|\psi) &= \left|\left\langle L_z^2 = 1 \mid L_z = 1\right\rangle\right|^2 + \left|\left\langle L_z^2 = 1 \mid L_z = 0\right\rangle\right|^2 + \left|\left\langle L_z^2 = 1 \mid L_z = -1\right\rangle\right|^2 \\
&= \frac{1}{4} + \frac{1}{2} = \frac{3}{4}
\end{aligned}$$

(f) A particle is in a state for which the probabilities are $P(L_z = 1) = 1/4$, $P(L_z = 0) = 1/2$ and $P(L_z = -1) = 1/4$. Convince yourself that the most general, normalized state with this property is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2}|L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}}|L_z = 0\rangle + \frac{e^{i\delta_3}}{2}|L_z = -1\rangle$$

We know that if $|\psi\rangle$ is a normalized state then the state $e^{i\theta}|\psi\rangle$ is a physically equivalent state. Does this mean that the factors $e^{i\delta_j}$ multiplying the L_z eigenstates are irrelevant? Calculate, for example, $P(L_x = 0)$.

Since the phase factor does not affect absolute values, we have, for

$$|\psi\rangle = \frac{e^{i\delta_1}}{2}|L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}}|L_z = 0\rangle + \frac{e^{i\delta_3}}{2}|L_z = -1\rangle$$

$$\begin{array}{l} P(L_z = 1|\psi) = |\langle L_z = 1 \mid \psi\rangle|^2 = \frac{1}{4} \\ P(L_z = 0|\psi) = |\langle L_z = 0 \mid \psi\rangle|^2 = \frac{1}{4} \\ P(L_z = -1|\psi) = |\langle L_z = -1 \mid \psi\rangle|^2 = \frac{1}{2} \end{array}$$

as before.

Phase factors (or really relative phases) matter, however, for some measurements. If I write $|\psi\rangle$ in the $|_x$ basis we get

$$|\psi\rangle = \frac{e^{i\delta_1} - e^{i\delta_3}}{2\sqrt{2}}|L_x = 0\rangle + ...$$

so that

$$\langle L_x = 0 \mid \psi\rangle = \frac{e^{i\delta_1} - e^{i\delta_3}}{2\sqrt{2}}$$

and hence

$$P(L_x = 0|\psi) = |\langle L_x = 0 \mid \psi\rangle|^2 = \left|\frac{e^{i\delta_1} - e^{i\delta_3}}{2\sqrt{2}}\right|^2 = \frac{1}{4}\left(1 - \cos\left(\delta_1 - \delta_3\right)\right)$$

so clearly relative phase matters.

7.7.8 A Spin-3/2 Particle

Consider a particle with spin angular momentum $j = 3/2$. The are four sublevels with this value of j, but different eigenvalues of j_z, $|m = 3/2\rangle$,$|m = 1/2\rangle$,$|m = -1/2\rangle$ and $|m = -3/2\rangle$.

We have

$$\hat{J}^2 |3/2, 3/2\rangle = \hbar^2(3/2)(3/2+1) |3/2, 3/2\rangle = 15\hbar^2/4 |3/2, 3/2\rangle$$
$$\hat{J}_z |3/2, 3/2\rangle = 3\hbar/2 |3/2, 3/2\rangle$$
$$\hat{J}^2 |3/2, 1/2\rangle = \hbar^2(3/2)(3/2+1) |3/2, 1/2\rangle = 15\hbar^2/4 |3/2, 1/2\rangle$$
$$\hat{J}_z |3/2, 1/2\rangle = \hbar/2 |3/2, 1/2\rangle$$
$$\hat{J}^2 |3/2, -1/2\rangle = \hbar^2(3/2)(3/2+1) |3/2, -1/2\rangle = 15\hbar^2/4 |3/2, -1/2\rangle$$
$$\hat{J}_z |3/2, -1/2\rangle = -\hbar/2 |3/2, -1/2\rangle$$
$$\hat{J}^2 |3/2, -3/2\rangle = \hbar^2(3/2)(3/2+1) |3/2, -3/2\rangle = 15\hbar^2/4 |3/2, -3/2\rangle$$
$$\hat{J}_z |3/2, -3/2\rangle = -3\hbar/2 |3/2, -3/2\rangle$$

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

$$\begin{aligned}
\hat{J}_+ |3/2, 3/2\rangle &= \hbar\left(\sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |-1/2\rangle \langle -3/2|\right) |3/2, 3/2\rangle \\
&= 0 = \hbar\sqrt{3/2(3/2+1) - 3/2(3/2+1)} |3/2, 3/2\rangle \\
\hat{J}_+ |3/2, 1/2\rangle &= \hbar\left(\sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |-1/2\rangle \langle -3/2|\right) |3/2, 1/2\rangle \\
&= \sqrt{3}\hbar |3/2, 3/2\rangle = \hbar\sqrt{3/2(3/2+1) - 1/2(1/2+1)} |3/2, 3/2\rangle \\
\hat{J}_+ |3/2, -1/2\rangle &= \hbar\left(\sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |-1/2\rangle \langle -3/2|\right) |3/2, -1/2\rangle \\
&= 2\hbar |3/2, 1/2\rangle = \hbar\sqrt{3/2(3/2+1) + 1/2(-1/2+1)} |3/2, 1/2\rangle \\
\hat{J}_+ |3/2, -3/2\rangle &= \hbar\left(\sqrt{3} |3/2\rangle \langle 1/2| + 2 |1/2\rangle \langle -1/2| + \sqrt{3} |-1/2\rangle \langle -3/2|\right) |3/2, -3/2\rangle \\
&= \sqrt{3}\hbar |3/2, -1/2\rangle = \hbar\sqrt{3/2(3/2+1) + 3/2(-3/2+1)} |3/2, -1/2\rangle
\end{aligned}$$

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

$$\hat{j}_- = (\hat{j}_+)^+ = \hbar\left(\sqrt{3}\,|3/2\rangle\langle 1/2| + 2\,|1/2\rangle\langle -1/2| + \sqrt{3}\,|-1/2\rangle\langle -3/2|\right)^+$$
$$= \hbar\left(\sqrt{3}\,|1/2\rangle\langle 3/2| + 2\,|-1/2\rangle\langle 1/2| + \sqrt{3}\,|-3/2\rangle\langle -1/2|\right)$$

(c) What are the matrix representations of $\hat{J}_\pm$, $\hat{J}_x$, $\hat{J}_y$, $\hat{J}_z$ and $\hat{J}^2$ in the J_z basis?

$\hat{J}^2$ and J_z are both diagonal

$$\hat{J}^2 = \frac{15}{4}\hbar^2\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad , \quad \hat{J}_z = \hbar\begin{pmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{pmatrix}$$

The other operators are not diagonal,

$$\hat{J}_+ = \hbar\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad , \quad \hat{J}_- = \hbar\begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

and

$$\hat{J}_x = \frac{\hat{J}_+ + \hat{J}_-}{2} = \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$
$$\hat{J}_y = \frac{\hat{J}_+ - \hat{J}_-}{2i} = \frac{\hbar}{2i}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 0 & 2 & 0 \\ 0 & -2 & 0 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 0 \end{pmatrix}$$

(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

$$|\psi\rangle = \frac{1}{2\sqrt{2}}\left(\sqrt{3}\,|3/2\rangle + = |1/2\rangle - |-1/2\rangle - \sqrt{3}\,|-3/2\rangle\right) = \frac{1}{2\sqrt{2}}\begin{pmatrix} \sqrt{3} \\ 1 \\ -1 \\ -\sqrt{3} \end{pmatrix}$$

in the standard basis. The state is normalized since

$$\langle \psi \mid \psi \rangle = \frac{1}{8}\begin{pmatrix} \sqrt{3} & 1 & -1 & -\sqrt{3} \end{pmatrix}\begin{pmatrix} \sqrt{3} \\ 1 \\ -1 \\ -\sqrt{3} \end{pmatrix} = \frac{1}{8}(3+1+1+3) = 1$$

We also have

$$\hat{J}_x \left|\psi\right\rangle = \frac{1}{2\sqrt{2}}\frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}\begin{pmatrix} \sqrt{3} \\ 1 \\ -1 \\ -\sqrt{3} \end{pmatrix} = \frac{\hbar}{4\sqrt{2}}\begin{pmatrix} \sqrt{3} \\ 1 \\ -1 \\ -\sqrt{3} \end{pmatrix}\left|\psi\right\rangle = \frac{\hbar}{2}\left|\psi\right\rangle$$

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

$$\begin{aligned} \hat{J}_x \left|\psi_{3/2}\right\rangle &= \tfrac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} \\ &= \tfrac{\hbar}{2}\begin{pmatrix} \sqrt{3}b \\ \sqrt{3}a + 2c \\ 2b + \sqrt{3}d \\ \sqrt{3}c \end{pmatrix}\left|\psi\right\rangle = \tfrac{3\hbar}{2}\left|\psi_{3/2}\right\rangle = \tfrac{3\hbar}{2}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} \end{aligned}$$

$$\begin{aligned} &\sqrt{3}b = 3a \\ &\sqrt{3}a + 2c = 3b \\ &2b + \sqrt{3}d = 3c \quad \Rightarrow b = c = \sqrt{3}a = \sqrt{3}d \quad \Rightarrow \left|\psi_{3/2}\right\rangle = \tfrac{1}{2\sqrt{2}}\begin{pmatrix} 1 \\ \sqrt{3} \\ \sqrt{3} \\ 1 \end{pmatrix} \end{aligned}$$

(f) Suppose the particle describes the nucleus of an atom, which has a magnetic moment described by the operator $\vec{\mu} = g_N \mu_N \vec{j}$, where g_N is the *g-factor* and μ_N is the so-called *nuclear magneton*. At time $t = 0$, the system is prepared in the state given in (c). A magnetic field, pointing in the y direction of magnitude B, is suddenly turned on. What is the evolution of $\left\langle \hat{j}_z \right\rangle$ as a function of time if

$$\hat{H} = -\hat{\mu} \cdot \vec{B} = -g_N \mu_N \hbar \vec{J} \cdot \vec{B}\hat{y} = -g_N \mu_N \hbar B \hat{J}_y$$

where $\mu_N = e\hbar/2Mc =$ nuclear magneton? You will need to use the identity we derived earlier

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

We suppose at $t = 0$ we are in the state $\left|\psi_{3/2}\right\rangle$, describing a positive nucleus with g-factor g_N. The time evolution of the state is given by

$$\left|\psi_{3/2}(t)\right\rangle = \hat{U}(t)\left|\psi_{3/2}\right\rangle = e^{-i\hat{H}t/\hbar}\left|\psi_{3/2}\right\rangle = e^{-i\alpha t\hat{J}_y}\left|\psi_{3/2}\right\rangle$$

where $\alpha = -g_N\mu_N B$.

Then the time evolution of $\left\langle \hat{J}_z \right\rangle$ is given by

$$\left\langle \hat{J}_z \right\rangle_t = \left\langle\psi_{3/2}\right| e^{i\alpha t\hat{J}_y}\hat{j}_z e^{-i\alpha t\hat{J}_y}\left|\psi_{3/2}\right\rangle \left|\psi\right\rangle$$

Now we have that

$$e^{x\hat{A}}\hat{B}e^{-x\hat{A}} = \hat{B} + \left[\hat{A},\hat{B}\right]x + \left[\hat{A},\left[\hat{A},\hat{B}\right]\right]\tfrac{x^2}{2} + \left[\hat{A},\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]\right]\tfrac{x^3}{6} + ...$$
$$\left[\hat{J}_i,\hat{J}_j\right] = i\varepsilon_{ijk}\hat{J}_k$$

or

$$\left[\hat{J}_x,\hat{J}_y\right] = i\hat{J}_z \quad , \quad \left[\hat{J}_y,\hat{J}_z\right] = i\hat{J}_x \quad , \quad \left[\hat{J}_z,\hat{J}_x\right] = i\hat{J}_y$$

Thus,

$$\begin{aligned}
e^{x\hat{J}_y}\hat{J}_z e^{-x\hat{J}_y} &= \hat{J}_z + \left[\hat{J}_y,\hat{J}_z\right]x + \left[\hat{J}_y,\left[\hat{J}_y,\hat{J}_z\right]\right]\tfrac{x^2}{2} + \left[\hat{J}_y,\left[\hat{J}_y,\left[\hat{J}_y,\hat{J}_z\right]\right]\right]\tfrac{x^3}{6} + ...\\
e^{x\hat{J}_y}\hat{J}_z e^{-x\hat{J}_y} &= \hat{J}_z + i\hat{J}_x x + \left[\hat{J}_y,i\hat{J}_x\right]\tfrac{x^2}{2} + \left[\hat{J}_y,\left[\hat{J}_y,i\hat{J}_x\right]\right]\tfrac{x^3}{6} + ...\\
e^{x\hat{J}_y}\hat{J}_z e^{-x\hat{J}_y} &= \hat{J}_z + i\hat{J}_x x + \hat{J}_z\tfrac{x^2}{2} + \left[\hat{J}_y,\hat{J}_z\right]\tfrac{x^3}{6} + ...\\
e^{x\hat{J}_y}\hat{J}_z e^{-x\hat{J}_y} &= \hat{J}_z + i\hat{J}_x x + \hat{J}_z\tfrac{x^2}{2} + i\hat{J}_x\tfrac{x^3}{6} + ... = \cos(\alpha t/\hbar)\hat{J}_z - \sin(\alpha t/\hbar)\hat{J}_x
\end{aligned}$$

where $x = i\alpha t/\hbar$. Therefore,

$$\begin{aligned}
\left\langle \hat{J}_z \right\rangle_t &= \left\langle\psi_{3/2}\right|\left(\cos(\alpha t)\hat{J}_z - \sin(\alpha t)\hat{J}_x\right)\left|\psi_{3/2}\right\rangle\\
&= \cos(\alpha t)\left\langle\psi_{3/2}\right|\hat{J}_z\left|\psi_{3/2}\right\rangle - \sin(\alpha t)\left\langle\psi_{3/2}\right|\hat{J}_x\left|\psi_{3/2}\right\rangle\left|\psi_{3/2}\right\rangle
\end{aligned}$$

Now

$$\begin{aligned}
\left\langle\psi_{3/2}\right|\hat{J}_z\left|\psi_{3/2}\right\rangle &= 0\\
\left\langle\psi_{3/2}\right|\hat{J}_x\left|\psi_{3/2}\right\rangle &= \tfrac{3\hbar}{2}
\end{aligned}$$

so that

$$\left\langle \hat{J}_z \right\rangle_t = \frac{3\hbar}{2}\sin g_N\mu_N Bt$$

7.7.9 Arbitrary directions

Method #1

(a) Using the $|z+\rangle$ and $|z-\rangle$ states of a spin 1/2 particle as a basis, set up and solve as a problem in matrix mechanics the eigenvalue/eigenvector problem for $S_n = \vec{S} \cdot \hat{n}$ where the spin operator is

$$\vec{S} = \hat{S}_x \hat{e}_x + \hat{S}_y \hat{e}_y + \hat{S}_z \hat{e}_z$$

and

$$\hat{n} = \sin\theta\cos\varphi \hat{e}_x + \sin\theta\sin\varphi \hat{e}_y + \cos\theta \hat{e}_z$$

(b) Show that the eigenstates may be written as

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

In the $\hat{\sigma}_z$ basis we have

$$\hat{S}_x = \tfrac{\hbar}{2}\hat{\sigma}_x = \tfrac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
$$\hat{S}_y = \tfrac{\hbar}{2}\hat{\sigma}_y = \tfrac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$
$$\hat{S}_z = \tfrac{\hbar}{2}\hat{\sigma}_z = \tfrac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Therefore,

$$\hat{S}_n = \hat{\vec{S}} \cdot \hat{n} = \left(\hat{S}_x \hat{e}_x + \hat{S}_y \hat{e}_y + \hat{S}_z \hat{e}_z\right) \cdot (\sin\theta\cos\varphi \hat{e}_x + \sin\theta\sin\varphi \hat{e}_y + \cos\theta \hat{e}_z)$$
$$= \hat{S}_x \sin\theta\cos\varphi + \hat{S}_y \sin\theta\sin\varphi + \hat{S}_z\cos\theta = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}$$

Eigenvalue/Eigenvector problem

$$\hat{S}_n |\psi\rangle = \lambda\frac{\hbar}{2}|\psi\rangle$$

or in matrix form

$$\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} \langle +\hat{z} \mid \psi\rangle \\ \langle -\hat{z} \mid \psi\rangle \end{pmatrix} = \lambda\begin{pmatrix} \langle +\hat{z} \mid \psi\rangle \\ \langle -\hat{z} \mid \psi\rangle \end{pmatrix}$$

which is two homogeneous equations in two unknowns $\langle \pm\hat{z} \mid \psi\rangle$. For a non-trivial solution, the determinant of the coefficients must vanish

$$\begin{vmatrix} \cos\theta - \lambda & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta - \lambda \end{vmatrix} = 0 = -\cos^2\theta - \sin^2\theta + \lambda^2 \to \lambda^2 = 1 \to \lambda = \pm 1$$

For $\lambda = +1$, we have

$$\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} \langle +\hat{z} \mid \psi\rangle \\ \langle -\hat{z} \mid \psi\rangle \end{pmatrix} = \begin{pmatrix} \langle +\hat{z} \mid \psi\rangle \\ \langle -\hat{z} \mid \psi\rangle \end{pmatrix}$$
$$(\cos\theta - 1)\langle +\hat{z} \mid \psi\rangle + e^{-i\varphi}\sin\theta\langle -\hat{z} \mid \psi\rangle = 0$$

and from normalization

$$|\langle +\hat{z} \mid \psi\rangle|^2 + |\langle -\hat{z} \mid \psi\rangle|^2 = 1$$

so that

$$\begin{aligned}
&|\langle +\hat{z} \mid \psi\rangle|^2 \left[1 - \left(\tfrac{1-\cos\theta}{\sin\theta}\right)^2\right] = 1 \\
&|\langle +\hat{z} \mid \psi\rangle|^2 = \tfrac{\sin^2\theta}{2(1-\cos\theta)} = \tfrac{(1-\cos\theta)(1+\cos\theta)}{2(1-\cos\theta)} = \tfrac{(1+\cos\theta)}{2} = \cos^2\tfrac{\theta}{2} \\
&\langle +\hat{z} \mid \psi\rangle = \cos\tfrac{\theta}{2}
\end{aligned}$$

and

$$\begin{aligned}
\langle -\hat{z} \mid \psi\rangle &= \frac{1-\cos\theta}{e^{-i\varphi}\sin\theta}\langle +\hat{z} \mid \psi\rangle = \frac{1-\cos\theta}{e^{-i\varphi}\sin\theta}\cos\frac{\theta}{2} \\
&= \frac{1-\cos\theta}{e^{-i\varphi}\sqrt{(1-\cos\theta)(1-\cos\theta)}}\sqrt{\frac{1+\cos\theta}{2}} \\
&= e^{i\varphi}\sqrt{\frac{1-\cos\theta}{2}} = e^{i\varphi}\sin\frac{\theta}{2}
\end{aligned}$$

so that

$$|\lambda = +1\rangle = \langle +\hat{z} \mid \psi\rangle\,|+\hat{z}\rangle + \langle -\hat{z} \mid \psi\rangle\,|-\hat{z}\rangle = \cos\frac{\theta}{2}\,|+\hat{z}\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|-\hat{z}\rangle = |+\hat{n}\rangle$$

Similarly, for $\lambda = -1$, we have

$$\begin{aligned}
&\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} \langle +\hat{z} \mid \psi\rangle \\ \langle -\hat{z} \mid \psi\rangle \end{pmatrix} = -\begin{pmatrix} \langle +\hat{z} \mid \psi\rangle \\ \langle -\hat{z} \mid \psi\rangle \end{pmatrix} \\
&(\cos\theta + 1)\,\langle +\hat{z} \mid \psi\rangle + e^{-i\varphi}\sin\theta\,\langle -\hat{z} \mid \psi\rangle = 0
\end{aligned}$$

and from normalization

$$|\langle +\hat{z} \mid \psi\rangle|^2 + |\langle -\hat{z} \mid \psi\rangle|^2 = 1$$

so that

$$\begin{aligned}
&|\langle +\hat{z} \mid \psi\rangle|^2 \left[1 + \left(\tfrac{1+\cos\theta}{\sin\theta}\right)^2\right] = 1 \\
&|\langle +\hat{z} \mid \psi\rangle|^2 = \tfrac{\sin^2\theta}{2(1+\cos\theta)} = \tfrac{(1-\cos\theta)(1+\cos\theta)}{2(1+\cos\theta)} = \tfrac{(1-\cos\theta)}{2} = \sin^2\tfrac{\theta}{2} \\
&\langle +\hat{z} \mid \psi\rangle = \sin\tfrac{\theta}{2}
\end{aligned}$$

and

$$\begin{aligned}
\langle -\hat{z} \mid \psi\rangle &= -\frac{1+\cos\theta}{e^{-i\varphi}\sin\theta}\langle +\hat{z} \mid \psi\rangle = -\frac{1+\cos\theta}{e^{-i\varphi}\sin\theta}\sin\frac{\theta}{2} \\
&= -\frac{1+\cos\theta}{e^{-i\varphi}\sqrt{(1-\cos\theta)(1-\cos\theta)}}\sqrt{\frac{1-\cos\theta}{2}} \\
&= -e^{i\varphi}\sqrt{\frac{1+\cos\theta}{2}} = -e^{i\varphi}\cos\frac{\theta}{2}
\end{aligned}$$

so that

$$|\lambda=-1\rangle = \langle +\hat{z} \mid \psi\rangle \,|+\hat{z}\rangle + \langle -\hat{z} \mid \psi\rangle \,|-\hat{z}\rangle = \sin\frac{\theta}{2}\,|+\hat{z}\rangle - e^{i\varphi}\cos\frac{\theta}{2}\,|-\hat{z}\rangle = |-\hat{n}\rangle$$

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 θ counterclockwise about the $y-$axis.

(a) Show that this rotation operator can be expressed in the form

$$\hat{R}(\theta\hat{e}_y) = \cos\frac{\theta}{2} - \frac{2i}{\hbar}\hat{S}_y\sin\frac{\theta}{2}$$

(b) Apply $\hat{R}$ to the states $|z+\rangle$ and $|z-\rangle$ to obtain the state $|\hat{n}+\rangle$ with $\varphi = 0$, that is, rotated by angle θ in the $x-z$ plane.

In the $\hat{S}_z$ basis

$$\hat{S}_y = \tfrac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \to (\hat{S}_y)^2 = \tfrac{\hbar^2}{4}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \tfrac{\hbar^2}{4}\hat{I}$$
$$\to (\hat{S}_y)^3 = \tfrac{\hbar^3}{8}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \tfrac{\hbar^2}{4}\hat{S}_y \to (\hat{S}_y)^4 = \tfrac{\hbar^4}{16}\hat{I} \text{ and so on ......}$$

This implies that

$$\begin{aligned}\hat{R}(\theta\hat{e}_y) = e^{-i\hat{S}_y\theta/\hbar} &= \hat{I} + \left(-\tfrac{i\theta}{\hbar}\right)\hat{S}_y + \tfrac{1}{2!}\left(-\tfrac{i\theta}{\hbar}\right)^2(\hat{S}_y)^2 \\ &\quad + \tfrac{1}{3!}\left(-\tfrac{i\theta}{\hbar}\right)^3(\hat{S}_y)^3 + \tfrac{1}{4!}\left(-\tfrac{i\theta}{\hbar}\right)^4(\hat{S}_y)^4 + ... \\ &= \hat{I} + \left(-\tfrac{i\theta}{\hbar}\right)\left(\tfrac{\hbar}{2}\right)\hat{\sigma}_y + \tfrac{1}{2!}\left(-\tfrac{i\theta}{\hbar}\right)^2\left(\tfrac{\hbar}{2}\right)^2\hat{I} + \tfrac{1}{3!}\left(-\tfrac{i\theta}{\hbar}\right)^3\left(\tfrac{\hbar}{2}\right)^3\hat{\sigma}_y \\ &\quad + \tfrac{1}{4!}\left(-\tfrac{i\theta}{\hbar}\right)^4\left(\tfrac{\hbar}{2}\right)^4\hat{I} + \tfrac{1}{5!}\left(-\tfrac{i\theta}{\hbar}\right)^5\left(\tfrac{\hbar}{2}\right)^5\hat{\sigma}_y + ... \\ &= \cos\tfrac{\theta}{2}\hat{I} - i\hat{\sigma}_y\sin\tfrac{\theta}{2}\end{aligned}$$

as expected from the general rule

$$e^{-i\alpha\hat{\sigma}\cdot\hat{n}} = \cos\alpha\hat{I} - i\hat{\sigma}\cdot\hat{n}\sin\alpha$$

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 $|-\hat{n}(\varphi=0)\rangle$.

7.7.10 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

$$\left|+\hat{z}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \hat{\sigma}_z \left|+\hat{z}\right\rangle = +\left|+\hat{z}\right\rangle \rightarrow \hat{S}_z \left|+\hat{z}\right\rangle = \frac{\hbar}{2}\hat{\sigma}_z \left|+\hat{z}\right\rangle = +\frac{\hbar}{2}\left|+\hat{z}\right\rangle$$

The eigenvectors of $\hat{\sigma}_x$ in the $\hat{\sigma}_z$ representation are

$$\left|\pm\hat{x}\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \rightarrow \hat{\sigma}_x \left|\pm\hat{x}\right\rangle = \pm\left|\pm\hat{x}\right\rangle$$

Expanding $\left|+\hat{z}\right\rangle$ in the $\hat{\sigma}_x$ states in the $\hat{\sigma}_z$ representation we have

$$\left|+\hat{z}\right\rangle = \frac{1}{\sqrt{2}}\left|+\hat{x}\right\rangle + \frac{1}{\sqrt{2}}\left|-\hat{x}\right\rangle$$

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

$$P(+\hbar/2) = \left|\langle +\hat{x} \mid +\hat{z}\rangle\right|^2 = \tfrac{1}{2}$$
$$P(-\hbar/2) = \left|\langle -\hat{x} \mid +\hat{z}\rangle\right|^2 = \tfrac{1}{2}$$

so that

$$\left\langle \hat{S}_x \right\rangle = \frac{\hbar}{2}P(+\hbar/2) - \frac{\hbar}{2}P(-\hbar/2) = 0$$

(c) If the axis defining the measured spin direction makes an angle θ 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 $\hat{S}_n = \hat{\vec{S}} \cdot \hat{n}$ are (see earlier problem) in the $\hat{\sigma}_z$ basis are

$$\left|+\hat{n}\right\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \quad , \quad \left|-\hat{n}\right\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}$$

with eigenvalues $+\hbar/2$ and $-\hbar/2$ respectively.

Therefore

$$\left|+\hat{z}\right\rangle = \cos\frac{\theta}{2}\left|+\hat{n}\right\rangle + \sin\frac{\theta}{2}\left|-\hat{n}\right\rangle$$

so that

$$P(+\hbar/2;\hat{n}) = \left|\langle +\hat{n} \mid +\hat{z}\rangle\right|^2 = \cos^2\tfrac{\theta}{2}$$
$$P(-\hbar/2;\hat{n}) = \left|\langle -\hat{n} \mid +\hat{z}\rangle\right|^2 = \sin^2\tfrac{\theta}{2}$$

(d) What is the expectation value of the spin measurement in (c)?

$$\left\langle \hat{S}_n \right\rangle = \frac{\hbar}{2}P(+\hbar/2) - \frac{\hbar}{2}P(-\hbar/2) = \frac{\hbar}{2}\left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right) = \frac{\hbar}{2}\cos\theta$$

7.7.11 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

$$\hat{Q} = A\frac{\hbar}{2}\hat{\sigma}_y + B\frac{\hbar}{2}\hat{\sigma}_z$$

$$\begin{aligned}\hat{Q}^2 &= \frac{\hbar^2}{4}\left(A^2\left(\hat{\sigma}_y\right)^2 + B^2\left(\hat{\sigma}_z\right)^2 + AB\left\{\hat{\sigma}_y, \hat{\sigma}_z\right\}\right) \\ &= \frac{\hbar^2}{4}\left(A^2(1) + B^2(1) + AB(0)\right) = \frac{\hbar^2}{4}\left(A^2 + B^2\right)\end{aligned}$$

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

$$\hat{Q} = A\frac{\hbar}{2}\hat{\sigma}_y + B\frac{\hbar}{2}\hat{\sigma}_z = A\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + B\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} B & -iA \\ iA & -B \end{pmatrix}$$

so that the characteristic equation is

$$\begin{aligned}&\begin{vmatrix} \frac{\hbar}{2}B - E & -i\frac{\hbar}{2}A \\ i\frac{\hbar}{2}A & -\frac{\hbar}{2}B - E \end{vmatrix} = 0 = \left(\left(\tfrac{\hbar B}{2}\right)^2 - E^2\right) - \left(\tfrac{\hbar A}{2}\right)^2 \\ &\rightarrow E_\pm = Q_\pm = \pm\tfrac{\hbar}{2}\sqrt{A^2 + B^2}\end{aligned}$$

To get the eigenvectors we use

$$\hat{Q}\left|\pm Q\right\rangle = \pm Q\left|\pm Q\right\rangle \rightarrow \frac{\hbar}{2}\begin{pmatrix} B & -iA \\ iA & -B \end{pmatrix}\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = \pm Q\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix}$$

or

$$\begin{aligned}\tfrac{\hbar}{2}Ba_\pm - i\tfrac{\hbar}{2}Ab_\pm &= Q_\pm a_\pm \\ i\tfrac{\hbar}{2}Aa_\pm - \tfrac{\hbar}{2}Bb_\pm &= Q_\pm b_\pm\end{aligned}$$

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

$$\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = N\begin{pmatrix} iA \\ B \mp \sqrt{A^2+B^2} \end{pmatrix} \text{ where } N = \text{ normalization factor}$$

Normalizing, we find that

$$\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = \frac{1}{\sqrt{A^2+\left(B \mp \sqrt{A^2+B^2}\right)^2}}\begin{pmatrix} iA \\ B \mp \sqrt{A^2+B^2} \end{pmatrix}$$

(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

$$|S_y = +\hbar/2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \end{pmatrix}$$

Therefore, the probability that $S_y = +\hbar/2$ in the states $|\pm Q\rangle$ is given by

$$\begin{aligned} P_\pm(S_y = +\hbar/2) &= \left|\langle S_y = +\hbar/2 \mid \pm Q\rangle\right|^2 \\ &= \left|\frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \end{pmatrix}^+ \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix}\right|^2 = \frac{1}{2}\left|ia_\pm + b_\pm\right|^2 \\ &= \frac{1}{2}\left(\left|a_\pm\right|^2 + \left|b_\pm\right|^2 - ia_\pm^* b_\pm + ia_\pm b_\pm^*\right) = \frac{1}{2}\left(1 - ia_\pm^* b_\pm + ia_\pm b_\pm^*\right) \end{aligned}$$

or

$$P_\pm(S_y = +\hbar/2) = \frac{1}{2}\left(1 - \frac{2A\left(B \mp \sqrt{A^2+B^2}\right)}{A^2+\left(B \mp \sqrt{A^2+B^2}\right)^2}\right)$$

7.7.12 Simultaneous Measurement

A beam of particles is subject to a simultaneous measurement of the angular momentum observables $\hat{L}^2$ and $\hat{L}_z$. The measurement gives pairs of values

$$(\ell, m) = (0,0) \quad and \quad (1,-1)$$

with probabilities 3/4 and 1/4 respectively.

(a) Reconstruct the state of the beam immediately before the measurements.

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 α is an arbitrary phase.

(b) The particles in the beam with $(\ell, m) = (1, -1)$ are separated out and subjected to a measurement of $\hat{L}_x$. What are the possible outcomes and their probabilities?

The possible outcomes will correspond to the common eigenvectors of L^2 , L_z,

$$|1, m_x = 1\rangle \quad , \quad |1, m_x = 0\rangle \quad , \quad |1, m_x = -1\rangle$$

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

$$C_0 = m_x\sqrt{2}C_1 = m_x\sqrt{2}C_{-1} \quad , \quad C_1 + C_{-1} = m_x\sqrt{2}C_0$$

Therefore, we are led to

$$\begin{array}{l} |1, m_x = 1\rangle = \frac{1}{2}\left(|1,1\rangle + \sqrt{2}|1,0\rangle + |1,-1\rangle\right) \\ |1, m_x = 0\rangle = \frac{1}{\sqrt{2}}\left(|1,1\rangle - |1,-1\rangle\right) \\ |1, m_x = -1\rangle = \frac{1}{2}\left(|1,1\rangle - \sqrt{2}|1,0\rangle + |1,-1\rangle\right) \end{array}$$

The inverse expression for the L_z eigenstates are

$$\begin{array}{l} |1,1\rangle = \frac{1}{\sqrt{2}}|1, m_x = 1\rangle + \frac{1}{2}|1, m_x = 0\rangle + |1, m_x = -1\rangle \\ |1,0\rangle = \frac{1}{\sqrt{2}}|1, m_x = 1\rangle - \frac{1}{\sqrt{2}}|1, m_x = -1\rangle \\ |1,-1\rangle = -\frac{1}{\sqrt{2}}|1, m_x = 1\rangle + \frac{1}{2}|1, m_x = 0\rangle + |1, m_x = -1\rangle \end{array}$$

From these states we can read off the probabilities:

$$P_{L_z=\pm\hbar} = \frac{1}{4} \quad , \quad P_{L_z=0} = \frac{1}{2}$$

(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

$$\psi_{\pm 1} = \sqrt{\frac{3}{8\pi}}\left(\pm\cos\theta - i\sin\varphi\sin\theta\right) \quad , \quad \psi_0 = -\sqrt{\frac{3}{4\pi}}\cos\varphi\sin\theta$$

7.7.13 Vector Operator

Consider a vector operator $\vec{V}$ that satisfies the commutation relation

$$[L_i, V_j] = i\hbar\varepsilon_{ijk}V_k$$

This is the definition of a *vector operator*.

(a) Prove that the operator $e^{-i\varphi L_x/\hbar}$ is a rotation operator corresponding to a rotation around the $x-$axis by an angle φ, by showing that

$$e^{-i\varphi L_x/\hbar}V_i e^{i\varphi L_x/\hbar} = R_{ij}(\varphi)V_j$$

where $R_{ij}(\varphi)$ is the corresponding rotation matrix.

Consider the operator

$$X_i = e^{-i\varphi L_x/\hbar}V_i e^{i\varphi L_x/\hbar}$$

as a function of φ and differentiate it with respect to φ. We get

$$\begin{aligned}
\frac{dX_i}{d\varphi} &= \left(\frac{d}{d\varphi}e^{-i\varphi L_x/\hbar}\right)V_i e^{i\varphi L_x/\hbar} + e^{-i\varphi L_x/\hbar}V_i\left(\frac{d}{d\varphi}e^{i\varphi L_x/\hbar}\right) \\
&= -\frac{i}{\hbar}e^{-i\varphi L_x/\hbar}L_x V_i e^{i\varphi L_x/\hbar} + \frac{i}{\hbar}e^{-i\varphi L_x/\hbar}L_x V_i e^{i\varphi L_x/\hbar} \\
&= -\frac{i}{\hbar}e^{-i\varphi L_x/\hbar}\left[L_x, V_i\right]e^{i\varphi L_x/\hbar} = -\frac{i}{\hbar}e^{-i\varphi L_x/\hbar}\left(i\hbar\varepsilon_{xij}V_j\right)e^{i\varphi L_x/\hbar} \\
&= \varepsilon_{xij}X_j
\end{aligned}$$

From this we obtain

$$\begin{aligned}
\tfrac{dX_x}{d\varphi} &= \varepsilon_{xxj}X_j = 0 \Rightarrow X_x(\varphi) = X_x(0) = V_x \\
\tfrac{dX_y}{d\varphi} &= \varepsilon_{xyj}X_j = X_z \\
\tfrac{dX_z}{d\varphi} &= \varepsilon_{xzj}X_j = -X_y
\end{aligned}$$

The last two equations give

$$\begin{aligned}
\tfrac{d^2X_y}{d\varphi^2} &= -X_y \Rightarrow X_y(\varphi) = X_y(0)\cos\varphi + X_z(0)\sin\varphi = V_y\cos\varphi + V_z\sin\varphi \\
\tfrac{d^2X_z}{d\varphi^2} &= -X_z \Rightarrow X_z(\varphi) = X_z(0)\cos\varphi - X_y(0)\sin\varphi = V_z\cos\varphi - V_y\sin\varphi
\end{aligned}$$

or

$$e^{-i\varphi L_x/\hbar}V_i e^{i\varphi L_x/\hbar} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} = \Re_{ij}V_j$$

where the matrix $\Re$ is a rotation matrix corresponding to a rotation around the $x-$axis by an angle φ.

(b) Prove that
$$e^{-i\varphi L_x}\left|\ell,m\right\rangle = \left|\ell,-m\right\rangle$$
Putting $\varphi=\pi$ in the expression from (a) we get
$$e^{-i\varphi L_x/\hbar}L_z e^{i\varphi L_x/\hbar} = \Re_{zj}L_j = \Re_{zz}L_z = -L_z$$
Acting on the rotated state with L_z we get
$$L_z e^{i\pi L_x/\hbar}\left|\ell,m\right\rangle = -e^{-i\pi L_x/\hbar}L_z\left|\ell,m\right\rangle = -\hbar m e^{-i\pi L_x/\hbar}\left|\ell,m\right\rangle$$
Thus,
$$e^{i\pi L_x/\hbar}\left|\ell,m\right\rangle = \left|\ell,-m\right\rangle$$

(c) Show that a rotation by π around the $z-$axis can also be achieved by first rotating around the $x-$axis by $\pi/2$, then rotating around the $y-$axis by π and, finally rotating back by $-\pi/2$ around the $x-$axis. In terms of rotation operators this is expressed by
$$e^{i\pi L_x/2\hbar}e^{-i\pi L_y/\hbar}e^{-i\pi L_x/2\hbar} = e^{-i\pi L_z/\hbar}$$
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
$$e^{-i\pi L_x/2\hbar}(L_y)^n e^{i\pi L_x/2\hbar} = e^{-i\pi L_x/2\hbar}L_y e^{i\pi L_x/2\hbar}e^{-i\pi L_x/2\hbar}L_y e^{i\pi L_x/2\hbar}..... = (L_z)^n$$
and finally
$$e^{-i\pi L_x/2\hbar}e^{-i\pi L_y/\hbar}e^{i\pi L_x/2\hbar} = e^{-i\pi L_z/\hbar}$$

7.7.14 Addition of Angular Momentum

Two atoms with $J_1=1$ and $J_2=2$ are coupled, with an energy described by $\hat{H}=\varepsilon\vec{J}_1\cdot\vec{J}_2$, $\varepsilon>0$. Determine all of the energies and degeneracies for the coupled system.

We have
$$\begin{aligned}\vec{J}=\vec{J}_1+\vec{J}_2 \Rightarrow \vec{J}_1\cdot\vec{J}_2 &= \frac{1}{2}\left(\vec{J}^2-\vec{J}_1^2-\vec{J}_2^3\right)\\ &= \frac{1}{2}\left(\vec{J}^2-\hbar^2 J_1(J_1+1)I-\hbar^2 J_2(J_2+1)I\right)\\ &= \frac{1}{2}\left(\hbar^2 J(J+1)\hat{I}-2\hbar^2\hat{I}-6\hbar^2\hat{I}\right)\\ &= \frac{\hbar^2}{2}\left(J(J+1)-8\right)\hat{I}\end{aligned}$$

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

$$J = J_1 + J_2, ..., |J_1 - J_2| = 3, 2, 1$$

Thus, the final configurations are

$J = 1 : |1,1\rangle, |1,0\rangle, |1,-1\rangle \Rightarrow E = -3\varepsilon\hbar^2$
$J = 2 : |2,2\rangle, |2,1\rangle, |2,0\rangle, |2,-1\rangle, |2,-2\rangle \Rightarrow E = -\varepsilon\hbar^2$
$J = 3 : |3,3\rangle, |3,2\rangle, |3,1\rangle, |3,0\rangle, |3,-1\rangle, |3,-2\rangle, |3,-3\rangle \Rightarrow E = 2\varepsilon\hbar^2$

7.7.15 Spin = 1 system

We now consider a spin = 1 system.

(a) Use the spin = 1 states $|1,1\rangle$, $|1,0\rangle$ and $|1,-1\rangle$ (eigenstates of $\hat{S}_z$) as a basis to form the matrix representation (3×3) of the angular momentum operators $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$, $\hat{S}^2$, $\hat{S}_+$, and $\hat{S}_-$. In the $|1,1\rangle$, $|1,0\rangle$ and $|1,-1\rangle$ or $|S,S_z\rangle$ 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,

$$\hat{S}_- = \hat{S}_+^+ = \sqrt{2}\hbar\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

and

$$\hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$
$$\hat{S}_y = \frac{\hat{S}_+ - \hat{S}_-}{2i} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

Finally,

$$\begin{aligned}
\hat{S}^2 &= \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 \\
&= \frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} + \frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix} + \hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
&= 2\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = 1(1+1)\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\end{aligned}$$

(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

$$\begin{vmatrix} -m & \sqrt{2}/2 & 0 \\ \sqrt{2}/2 & -m & \sqrt{2}/2 \\ 0 & \sqrt{2}/2 & -m \end{vmatrix} = 0 = -m^3 + m \to m = 0, \pm 1$$

as expected. Substituting $m = 1$ into the eigenvalue equation, we get

$$\frac{\sqrt{2}}{2}b = a \quad , \quad \frac{\sqrt{2}}{2}(a+c) = b \quad , \quad \frac{\sqrt{2}}{2}b = c$$

so that

$$\begin{aligned}
&a = c \quad , \quad b = \sqrt{2}a \\
&\to |1,1\rangle_x = \tfrac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \tfrac{1}{2}|1,1\rangle + \tfrac{\sqrt{2}}{2}|1,0\rangle + \tfrac{1}{2}|1,-1\rangle
\end{aligned}$$

In a similar manner, we have for $m = 0$

$$\begin{aligned}
&b = 0 \quad , \quad a + c = 0 \\
&\to |1,0\rangle_x = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \tfrac{1}{\sqrt{2}}|1,1\rangle - \tfrac{1}{\sqrt{2}}|1,-1\rangle
\end{aligned}$$

and for $m = -1$

$$\begin{aligned}
&\tfrac{\sqrt{2}}{2}b = -a \quad , \quad \tfrac{\sqrt{2}}{2}(a+c) = -b \quad , \quad \tfrac{\sqrt{2}}{2}b = -c \\
&|1,-1\rangle_x = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \tfrac{1}{2}|1,1\rangle - \tfrac{\sqrt{2}}{2}|1,0\rangle + \tfrac{1}{2}|1,-1\rangle
\end{aligned}$$

(c) A spin = 1 particle is in the state

$$|\psi\rangle = \frac{1}{\sqrt{14}}\begin{pmatrix} 1 \\ 2 \\ 3i \end{pmatrix}$$

in the $\hat{S}_z$ basis.

$$|\psi\rangle = \begin{pmatrix} \langle 1,1 \mid \psi\rangle \\ \langle 1,0 \mid \psi\rangle \\ \langle 1,-1 \mid \psi\rangle \end{pmatrix} = \frac{1}{\sqrt{14}}\begin{pmatrix} 1 \\ 2 \\ 3i \end{pmatrix} \quad \text{inthe}\hat{S}_z\text{basis}$$

(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 $\left\langle \hat{S}_z \right\rangle$?

$$\begin{aligned} P(S_z = +\hbar) &= |\langle 1,1 \mid \psi\rangle|^2 = \left|\tfrac{1}{\sqrt{14}}\right|^2 = \tfrac{1}{14} \\ P(S_z = 0) &= |\langle 1,0 \mid \psi\rangle|^2 = \left|\tfrac{2}{\sqrt{14}}\right|^2 = \tfrac{2}{7} \\ P(S_z = -\hbar) &= |\langle 1,-1 \mid \psi\rangle|^2 = \left|\tfrac{3i}{\sqrt{14}}\right|^2 = \tfrac{9}{14} \end{aligned}$$

$$\langle S_z\rangle = \sum_{S_z} S_z P(S_z) = \hbar\left(\frac{1}{14}\right) + 0\left(\frac{2}{7}\right) - \hbar\left(\frac{9}{14}\right) = -\frac{4}{7}\hbar$$

(2) What is $\left\langle \hat{S}_x \right\rangle$ in this state?

$$\langle S_x\rangle = \langle\psi|\, \hat{S}_x\, |\psi\rangle = \frac{1}{\sqrt{14}}(1,2,-3i)\,\frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix} 1 \\ 2 \\ 3i \end{pmatrix} = \frac{\sqrt{2}}{7}\hbar$$

(3) What is the probability that a measurement of $\hat{S}_x$ will yield the value $\hbar$ for this state?

$$|1,1\rangle_x = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2}|1,1\rangle + \frac{\sqrt{2}}{2}|1,0\rangle + \frac{1}{2}|1,-1\rangle$$

Therefore,

$$\begin{aligned} {}_x\langle 1,1 \mid \psi\rangle &= \left(\frac{1}{2}\langle 1,1| + \frac{\sqrt{2}}{2}\langle 1,0| + \frac{1}{2}\langle 1,-1|\right)\frac{1}{\sqrt{14}}\left(|1,1\rangle + 2\,|1,0\rangle + 3i\,|1,-1\rangle\right) \\ &= \frac{1}{2}\frac{1}{\sqrt{14}}\left(1 + 2\sqrt{2} + 3i\right) \end{aligned}$$

and

$$P(S_x = +\hbar) = |_x \langle 1,1 \mid \psi\rangle|^2 = \left| \frac{1}{2}\frac{1}{\sqrt{14}}\left(1 + 2\sqrt{2} + 3i\right)\right|^2$$
$$= \frac{1}{56}\left(1 + 4\sqrt{2} + 8 + 9\right) = \frac{1}{28}\left(9 + 2\sqrt{2}\right)$$

(d) A particle with spin = 1 has the Hamiltonian

$$\hat{H} = A\hat{S}_z + \frac{B}{\hbar}\hat{S}_x^2$$

(1) Calculate the energy levels of this system.

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

$$\begin{vmatrix} A\hbar + B\hbar/2 - E & 0 & B\hbar/2 \\ 0 & B\hbar - E & 0 \\ B\hbar/2 & 0 & -A\hbar + B\hbar/2 - E \end{vmatrix} = 0$$

or

$$(B\hbar - E)\,(A\hbar + B\hbar/2 - E)\,(-A\hbar + B\hbar/2 - E) - (B\hbar - E)\,(B\hbar/2)\,(B\hbar/2) = 0$$
$$(B\hbar - E)\left((B\hbar/2 - E)^2 - (A\hbar)^2 - (B\hbar/2)^2\right) = 0$$

so that

$$E_0 = \hbar B \;\;,\;\; E_\pm = \hbar\frac{B}{2} \pm \sqrt{\hbar^2 A^2 + \frac{\hbar^2 B^2}{4}}$$

We now determine the eigenvectors.

For $E_0 = \hbar B = B'$

$$\hbar \begin{pmatrix} A + B/2 & 0 & B/2 \\ 0 & B & 0 \\ B/2 & 0 & -A + B/2 \end{pmatrix} \begin{pmatrix} a_0 \\ b_0 \\ c_0 \end{pmatrix} = \hbar B \begin{pmatrix} a_0 \\ b_0 \\ c_0 \end{pmatrix}$$
$$\to a_0 = c_0 = 0\ ,\ b_0 = 1 \to |E_0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

For $E_+ = \frac{\hbar}{2}\left(B + \sqrt{4A^2 + B^2}\right)$

$$\hbar \begin{pmatrix} A + B/2 & 0 & B/2 \\ 0 & B & 0 \\ B/2 & 0 & -A + B/2 \end{pmatrix} \begin{pmatrix} a_+ \\ b_+ \\ c_+ \end{pmatrix} = \lambda_+ \hbar \begin{pmatrix} a_+ \\ b_+ \\ c_+ \end{pmatrix}$$
$$= \frac{\hbar}{2}\left(B + \sqrt{4A^2 + B^2}\right)\begin{pmatrix} a_+ \\ b_+ \\ c_+ \end{pmatrix}$$

$$\begin{aligned}
&\left(A+\tfrac{B}{2}\right)a_+ + \tfrac{B}{2}c_+ = \lambda_+ a_+ \\
&Bb_+ = \lambda_+ b_+ \rightarrow b_+ = 0 \\
&\tfrac{B}{2}a_+ + \left(-A+\tfrac{B}{2}\right)c_+ = \lambda_+ c_+ \\
&a_+^2 + c_+^2 = 1
\end{aligned}$$

Then,

$$\begin{aligned}
&\tfrac{a_+}{c_+} = -\tfrac{\frac{B}{2}}{A+\frac{B}{2}-\lambda_+} = -\tfrac{B}{2A-\sqrt{4A^2+B^2}} = -\tfrac{B}{2A-\omega} \quad , \quad \omega = \sqrt{4A^2+B^2} \\
&a_+^2 + c_+^2 = 1 \rightarrow a_+ = \tfrac{B}{\sqrt{B^2+(\omega-2A)^2}} \quad , \quad c_+ = \tfrac{\omega-2A}{\sqrt{B^2+(\omega-2A)^2}} \\
&\rightarrow |E_+\rangle = \tfrac{1}{\sqrt{B^2+(\omega-2A)^2}} \begin{pmatrix} B \\ 0 \\ \omega-2A \end{pmatrix}
\end{aligned}$$

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 $\hat{S}_x$ with eigenvalue $\hbar$, calculate the expectation value of the spin $\left\langle \hat{S}_Z \right\rangle$ at time t.

Now

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle$$

and

$$|\psi(0)\rangle = |S_z = +\hbar\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{B^2+(\omega-2A)^2}} \left(B\,|E_+\rangle + (\omega-2A)\,|E_-\rangle\right)$$

so that

$$\begin{aligned}
|\psi(t)\rangle &= \frac{1}{\sqrt{B^2+(\omega-2A)^2}} \left(Be^{-i\hat{H}t/\hbar}\,|E_+\rangle + (\omega-2A)e^{-i\hat{H}t/\hbar}\,|E_-\rangle\right) \\
&= \frac{1}{\sqrt{B^2+(\omega-2A)^2}} \left(Be^{-iE_+t/\hbar}\,|E_+\rangle + (\omega-2A)e^{-iE_-t/\hbar}\,|E_-\rangle\right)
\end{aligned}$$

Now

$$\begin{aligned}
\hat{S}_z\,|E_+\rangle &= \tfrac{1}{\sqrt{B^2+(\omega-2A)^2}} \begin{pmatrix} B \\ 0 \\ -(\omega-2A) \end{pmatrix} \\
\hat{S}_z\,|E_-\rangle &= \tfrac{1}{\sqrt{B^2+(\omega-2A)^2}} \begin{pmatrix} (\omega-2A) \\ 0 \\ B \end{pmatrix}
\end{aligned}$$

Thus,

$$
\begin{aligned}
\langle S_z \rangle_t &= \langle \psi(t) | \hat{S}_z | \psi(t) \rangle \\
&= \frac{1}{\sqrt{B^2 + (\omega - 2A)^2}} \begin{pmatrix} Be^{iE_+ t/\hbar} \langle E_+ | \\ +(\omega - 2A) e^{iE_- t/\hbar} \langle E_- | \end{pmatrix} \\
&\quad \times \frac{1}{B^2 + (\omega - 2A)^2} \begin{pmatrix} Be^{-iE_+ t/\hbar} \begin{pmatrix} B \\ 0 \\ -(\omega - 2A) \end{pmatrix} \\ +(\omega - 2A) e^{-iE_- t/\hbar} \begin{pmatrix} (\omega - 2A) \\ 0 \\ B \end{pmatrix} \end{pmatrix}
\end{aligned}
$$

After lots of algebra, we find

$$
\langle S_z \rangle_t = \frac{1}{(B^2 + (\omega - 2A)^2)^2} \left((B^2 + (\omega - 2A)^2)^2 + 4B^2 (\omega - 2A)^2 \cos\left(\frac{E_+ - E_-}{\hbar} t \right) \right)
$$

Some limits:

(a) Let $B \to 0$, $\omega \to 2A$. We find $\langle S_z \rangle_t = \hbar =$ constant since

$$
\left[\hat{H}(B = 0), \hat{S}_z \right] = 0
$$

(b) Let $A \to 0$, $\omega \to B$. We find

$$
\langle S_z \rangle_t = \hbar \cos\left(\frac{E_+ - E_-}{\hbar} t \right) = \hbar \cos\left(\frac{\hbar B - 0}{\hbar} t \right) = \hbar \cos(Bt)
$$

which corresponds to precession.

7.7.16 Deuterium Atom

Consider a deuterium atom (composed of a nucleus of spin = 1 and an electron). The electronic angular momentum is $\vec{J} = \vec{L} + \vec{S}$, where $\vec{L}$ is the orbital angular momentum of the electron and $\vec{S}$ is its spin. The total angular momentum of the atom is $\vec{F} = \vec{J} + \vec{I}$, where $\vec{I}$ is the nuclear spin. The eigenvalues of $\hat{J}^2$ and $\hat{F}^2$ are $J(J+1)\hbar^2$ and $F(F+1)\hbar^2$ respectively.

(a) What are the possible values of the quantum numbers J and F for the deuterium atom in the $1s(L = 0)$ ground state?

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

$$
F = J + I, ... |J - I| = 3/2 \ , \ 1/2
$$

(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

$$F = 5/2, 3/2, 1/2$$

7.7.17 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

$$Y_1^{\pm 1} = \mp \left(\frac{3}{4\pi}\right)^{1/2} \frac{x \pm iy}{\sqrt{2}r} \quad , \quad Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \frac{z}{r}$$

$$Y_1^{\pm 1} = \mp\sqrt{\tfrac{3}{8\pi}} e^{\pm i\phi} \sin\theta = \mp\sqrt{\tfrac{3}{8\pi}} \tfrac{x \pm iy}{r}$$
$$Y_1^0 = \sqrt{\tfrac{3}{4\pi}} \cos\theta = \sqrt{\tfrac{3}{4\pi}} \tfrac{z}{r}$$

or

$$Y_1^{-1} - Y_1^{+1} = 2\sqrt{\tfrac{3}{8\pi}} \tfrac{x}{r}$$
$$-(Y_1^{-1} + Y_1^{+1}) = 2i\sqrt{\tfrac{3}{8\pi}} \tfrac{y}{r}$$

(b) Using this result, show that for a particle described by ψ above

$$P(L_z = 0) = 2/3\ ,\ P(L_z = \hbar) = 1/6\ ,\ P(L_z = -\hbar) = 1/6$$

Thus, we have

$$\psi = N(x + y + 2z)e^{-\alpha r} = Nf(r) \left(\frac{1+i}{\sqrt{2}} Y_1^{-1} - \frac{1-i}{\sqrt{2}} Y_1^{+1} + 2Y_1^0\right)$$

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,

$$\begin{aligned} P(L_z = 0|\psi) &= |\langle 1,0 \mid \psi\rangle|^2 = \tfrac{1}{6}\left|\tfrac{1+i}{\sqrt{2}}\right|^2 = \tfrac{1}{6} \\ P(L_z = +1|\psi) &= |\langle 1,1 \mid \psi\rangle|^2 = \tfrac{1}{6}\left|\tfrac{1-i}{\sqrt{2}}\right|^2 = \tfrac{1}{6} \\ P(L_z = -1|\psi) &= |\langle 1,-1 \mid \psi\rangle|^2 = \tfrac{1}{6}4 = \tfrac{2}{3} \end{aligned}$$

7.7.18 Spin in Magnetic Field

Suppose that we have a spin$-1/2$ particle interacting with a magnetic field via the Hamiltonian

$$\hat{H} = \begin{cases} -\vec{\mu}\cdot\vec{B}\ ,\ \vec{B} = B\hat{e}_z & 0 \le t < T \\ -\vec{\mu}\cdot\vec{B}\ ,\ \vec{B} = B\hat{e}_y & T \le t < 2T \end{cases}$$

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 $0 \le t < T$ we have

$$\hat{H} = -\hbar\omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

so that the Schrodinger equation becomes

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = i\hbar\begin{pmatrix} \dot{\alpha} \\ \dot{\beta} \end{pmatrix} = \hat{H}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -\hbar\omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -\hbar\omega\begin{pmatrix} \alpha \\ -\beta \end{pmatrix}$$

or

$$\begin{aligned} \dot{\alpha} &= i\omega\alpha \to \alpha(t) = Ae^{i\omega t} \\ \dot{\beta} &= -i\omega\beta \to \beta(t) = Be^{-i\omega t} \end{aligned}$$

The initial state (at $t = 0$) is

$$|\psi(0)\rangle = |x+\rangle = \frac{1}{\sqrt{2}}(|z+\rangle + |z-\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

so that

$$\alpha(0) = \frac{1}{\sqrt{2}} = A \quad , \quad \beta(0) = \frac{1}{\sqrt{2}} = B$$

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

$$\begin{aligned} &\dot{\alpha} = \omega\beta \rightarrow \ddot{\alpha} = \omega\dot{\beta} = -\omega^2\alpha \rightarrow \alpha(t) = c_1 e^{i\omega t} + c_2 e^{-i\omega t} \\ &\dot{\beta} = -\omega\alpha \rightarrow \ddot{\beta} = -\omega\dot{\alpha} = -\omega^2\beta \rightarrow \beta(t) = c_3 e^{i\omega t} + c_4 e^{-i\omega t} \end{aligned}$$

Now

$$\begin{aligned} &\dot{\alpha} = \omega\beta \rightarrow ic_1 = c_3 \quad , -ic_2 = c_4 \\ &\dot{\beta} = -\omega\alpha \rightarrow ic_3 = -c_1 \quad , -ic_4 = -c_2 \end{aligned}$$

so that

$$c_3 = ic_1 \text{ and } c_4 = -ic_2$$

and

$$\begin{aligned} \alpha(t) &= c_1 e^{i\omega t} + c_2 e^{-i\omega t} \\ \beta(t) &= i(c_1 e^{i\omega t} - c_2 e^{-i\omega t}) \end{aligned}$$

The initial state (at $t = T$) is

$$|\psi(T)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega T} \\ e^{-i\omega T} \end{pmatrix}$$

so that

$$\begin{aligned} \alpha(T) &= c_1 e^{i\omega T} + c_2 e^{-i\omega T} = \tfrac{1}{\sqrt{2}} e^{i\omega T} \\ \beta(T) &= i(c_1 e^{i\omega T} - c_2 e^{-i\omega T}) = \tfrac{1}{\sqrt{2}} e^{-i\omega T} \end{aligned}$$

or

$$\begin{aligned} c_1 e^{i\omega T} + c_2 e^{-i\omega T} &= \tfrac{1}{\sqrt{2}} e^{i\omega T} \\ c_1 e^{i\omega T} - c_2 e^{-i\omega T} &= -\tfrac{i}{\sqrt{2}} e^{-i\omega T} \end{aligned}$$

and

$$\begin{aligned} 2c_1 e^{i\omega T} &= \tfrac{1}{\sqrt{2}}\left(e^{i\omega T} - ie^{-i\omega T}\right) \\ 2c_2 e^{-i\omega T} &= \tfrac{1}{\sqrt{2}}\left(e^{i\omega T} + ie^{-i\omega T}\right) \end{aligned}$$

Finally, for $T \leq t \leq 2T$

$$
\begin{aligned}
|\psi(t)\rangle &= \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} c_1 e^{i\omega t} + c_2 e^{-i\omega t} \\ i(c_1 e^{i\omega t} - c_2 e^{-i\omega t}) \end{pmatrix} \\
&= \begin{pmatrix} \left(\frac{1}{2\sqrt{2}} e^{-i\omega T}\left(e^{i\omega T} - ie^{-i\omega T}\right)\right) e^{i\omega t} + \left(\frac{1}{2\sqrt{2}} e^{i\omega T}\left(e^{i\omega T} + ie^{-i\omega T}\right)\right) e^{-i\omega t} \\ \left(\frac{i}{2\sqrt{2}} e^{-i\omega T}\left(e^{i\omega T} - ie^{-i\omega T}\right)\right) e^{i\omega t} - \left(\frac{i}{2\sqrt{2}} e^{i\omega T}\left(e^{i\omega T} + ie^{-i\omega T}\right)\right) e^{-i\omega t} \end{pmatrix}
\end{aligned}
$$

Now, we need

$$
\begin{aligned}
&\langle S_x = + \mid \psi(2T)\rangle \\
&= \frac{1}{\sqrt{2}}(1,1) \begin{pmatrix} \left(\frac{1}{2\sqrt{2}} e^{-i\omega T}\left(e^{i\omega T} - ie^{-i\omega T}\right)\right) e^{2i\omega T} + \left(\frac{1}{2\sqrt{2}} e^{i\omega T}\left(e^{i\omega T} + ie^{-i\omega T}\right)\right) e^{-2i\omega T} \\ \left(\frac{i}{2\sqrt{2}} e^{-i\omega T}\left(e^{i\omega T} - ie^{-i\omega T}\right)\right) e^{2i\omega T} - \left(\frac{i}{2\sqrt{2}} e^{i\omega T}\left(e^{i\omega T} + ie^{-i\omega T}\right)\right) e^{-2i\omega T} \end{pmatrix} \\
&= \frac{1}{4}\left(\left(e^{2i\omega T} - i\right) + \left(1 + ie^{-2i\omega T}\right) + i\left(e^{2i\omega T} - i\right) - i\left(1 + ie^{-2i\omega T}\right)\right) \\
&= \frac{1}{4}\left((1+i)(e^{2i\omega T} + e^{-2i\omega T}) + 2(1-i)\right)
\end{aligned}
$$

so that

$$
\begin{aligned}
Prob &= \frac{1}{16}\left((2 + 2\cos 2\omega T)^2 + (2 - 2\cos 2\omega T)^2\right) \\
&= \frac{1}{16}\left(8 + 8\cos^2 2\omega T\right) = \frac{1}{2}\left(1 + \cos^2 2\omega T\right)
\end{aligned}
$$

(2) Using the time development operator (using operator algebra)

During the time interval $0 \leq t < T$ we have

$$
\hat{H} = -\hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
$$

The eigenvectors and eigenvalues of $\hat{H}$ are

$$
|z+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow E_+ = -\hbar\omega \quad , \quad |z-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow E_- = +\hbar\omega
$$

Initially,

$$
|\psi(0)\rangle = |x+\rangle = \frac{1}{\sqrt{2}}\left(|z+\rangle + |z-\rangle\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}
$$

Therefore,

$$
|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle = e^{-i\hat{H}t/\hbar}\frac{1}{\sqrt{2}}\left(|z+\rangle + |z-\rangle\right) = \frac{1}{\sqrt{2}}\left(e^{i\omega t}\,|z+\rangle + e^{-i\omega t}\,|z-\rangle\right)
$$

so that

$$
|\psi(T)\rangle = \frac{1}{\sqrt{2}}\left(e^{i\omega T}\,|z+\rangle + e^{-i\omega T}\,|z-\rangle\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega T} \\ e^{-i\omega T} \end{pmatrix}
$$

as in part (1).

Now during the time interval $T \leq t \leq 2T$ we have

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

$$\begin{aligned} |\psi(T)\rangle &= \frac{1}{\sqrt{2}} \left(e^{i\omega T} |z+\rangle + e^{-i\omega T} |z-\rangle \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega T} \\ e^{-i\omega T} \end{pmatrix} \\ &= a |y+\rangle + b |y-\rangle = \frac{a}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} + \frac{b}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \end{aligned}$$

or

$$a + b = e^{i\omega T} \quad , \quad i(a-b) = e^{-i\omega T}$$

or

$$\begin{aligned} 2a &= e^{i\omega T} - ie^{-i\omega T} \\ 2b &= e^{i\omega T} + ie^{-i\omega T} \end{aligned}$$

so that

$$|\psi(t)\rangle = e^{-i\hat{H}(t-T)/\hbar} \left(a |y+\rangle + b |y-\rangle \right) = ae^{i\omega(t-T)} |y+\rangle + be^{-i\omega(t-T)} |y-\rangle$$

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,

$$\begin{aligned} &\langle S_x = + \mid \psi(2T)\rangle \\ &= \frac{1}{\sqrt{2}} (1,1) \frac{1}{2\sqrt{2}} \left((e^{i\omega T} - ie^{-i\omega T})e^{i\omega T} \begin{pmatrix} 1 \\ i \end{pmatrix} + (e^{i\omega T} + ie^{-i\omega T})e^{-i\omega T} \begin{pmatrix} 1 \\ -i \end{pmatrix} \right) \\ &= \frac{1}{2} \left((1-i) + (1+i) \cos 2\omega T \right) \end{aligned}$$

and

$$\begin{aligned} Prob &= \frac{1}{4} \left((1 + \cos 2\omega T)^2 + (1 - \cos 2\omega T)^2 \right) \\ &= \frac{1}{4} \left(2 + 2\cos^2 2\omega T \right) = \frac{1}{2} \left(1 + \cos^2 2\omega T \right) \end{aligned}$$

as in part (1).

(3) Using the density operator formalism.

The initial system density operator is

$$\begin{aligned} \hat{\rho} &= |\psi(0)\rangle \langle\psi(0)| = |x+\rangle \langle x+) \\ &= \frac{1}{2} \left(|z+\rangle \langle z+| + |z+\rangle \langle z-| + |z-\rangle \langle z+| + |z-\rangle \langle z-| \right) = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{aligned}$$

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

$$\begin{aligned}
\begin{pmatrix} \dot{a} & \dot{b} \\ \dot{c} & \dot{d} \end{pmatrix} &= i\omega\left[\hat{\sigma}_z, \hat{\rho}(t)\right] \\
&= i\omega\left(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix} - \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right) \\
&= i\omega\begin{pmatrix} 0 & 2b \\ -2c & 0 \end{pmatrix}
\end{aligned}$$

so that

$$\begin{aligned}
&\dot{a} = 0 \to a(t) = a(0) = \tfrac{1}{2} \\
&\dot{d} = 0 \to d(t) = d(0) = \tfrac{1}{2} \\
&\dot{b} = 2i\omega b \to b(t) = \tfrac{1}{2}e^{2i\omega t} \\
&\dot{c} = -2i\omega c \to c(t) = \tfrac{1}{2}e^{-2i\omega t}
\end{aligned}$$

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

$$\begin{aligned}
\begin{pmatrix} \dot{a} & \dot{b} \\ \dot{c} & \dot{d} \end{pmatrix} &= i\omega\left[\hat{\sigma}_y, \hat{\rho}(t)\right] \\
&= i\omega\left(\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix} - \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\right) \\
&= -\omega\begin{pmatrix} -(b+c) & (a-d) \\ (a-d) & (b+c) \end{pmatrix}
\end{aligned}$$

so that

$$\dot{a} = \omega(b+c)\ ,\ a(T) = \tfrac{1}{2} \quad , \quad \dot{b} = -\omega(a-d)\ ,\ b(T) = \tfrac{1}{2}e^{2i\omega T}$$
$$\dot{c} = -\omega(a-d)\ ,\ c(T) = \tfrac{1}{2}e^{-2i\omega T} \quad , \quad \dot{d} = -\omega(b+c)\ ,\ d(T) = \tfrac{1}{2}$$

These equations say that

$$\dot{a} = -\dot{d} \to a = -d + G_1$$
$$\dot{b} = \dot{c} \to b = c + G_2$$

The boundary conditions then give

$$a(T) = -d(T) + G_1 \to G_1 = a(T) + d(T) = 1$$
$$b(T) = c(T) + G_2 \to G_2 = b(T) - c(T) = \tfrac{1}{2}e^{2i\omega T} - \tfrac{1}{2}e^{-2i\omega T} = i\sin 2\omega T$$

so that

$$a(t) = -d(t) + 1$$
$$b(t) = c(t) + i\sin 2\omega T$$

Therefore, we have the equations

$$\dot{a} = \omega(2b - i\sin 2\omega T)\ ,\ a(T) = \frac{1}{2} \quad , \quad \dot{b} = -\omega(2a-1)\ ,\ b(T) = \frac{1}{2}e^{2i\omega T}$$

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

$$a(t) = \mathrm{Re}^{2i\omega t} + Se^{-2i\omega t} + \tfrac{1}{2}$$
$$b(t) = Ue^{2i\omega t} + Ve^{-2i\omega t} + \tfrac{i}{2}\sin 2\omega T$$

In order for the equations to be consistent we must have

$$\dot{a} = \omega(2b - i\sin 2\omega T)$$
$$2i\omega\left(\mathrm{Re}^{2i\omega t} - Se^{-2i\omega t}\right) = 2\omega\left(Ue^{2i\omega t} + Ve^{-2i\omega t} + \tfrac{i}{2}\sin 2\omega T\right) - i\sin 2\omega T$$
$$i\left(\mathrm{Re}^{2i\omega t} - Se^{-2i\omega t}\right) = \left(Ue^{2i\omega t} + Ve^{-2i\omega t}\right)$$

or

$$iR = U \text{ and } -iS = V$$

Similarly, we must have

$$\dot{b} = -\omega(2a-1)$$
$$2i\omega\left(Ue^{2i\omega t} - Ve^{-2i\omega t}\right) = -2\omega\left(\mathrm{Re}^{2i\omega t} + Se^{-2i\omega t}\right)$$
$$\left(Ue^{2i\omega t} - Ve^{-2i\omega t}\right) = i\left(\mathrm{Re}^{2i\omega t} + Se^{-2i\omega t}\right)$$

or

$$iR = U \text{ and } -iS = V$$

which is identical to the above result.

So we have

$$a(t) = \mathrm{R}e^{2i\omega t} + Se^{-2i\omega t} + \tfrac{1}{2}$$
$$b(t) = i\mathrm{R}e^{2i\omega t} - iSe^{-2i\omega t} + \tfrac{i}{2}\sin 2\omega T$$

Now the boundary conditions are

$$a(T) = \tfrac{1}{2} = \mathrm{R}e^{2i\omega T} + Se^{-2i\omega T} + \tfrac{1}{2}$$
$$\mathrm{R}e^{2i\omega T} + Se^{-2i\omega T} = 0$$
$$b(T) = \tfrac{1}{2}e^{2i\omega T} = i\mathrm{R}e^{2i\omega T} - iSe^{-2i\omega T} + \tfrac{i}{2}\sin 2\omega T$$

$$\begin{aligned}\mathrm{R}e^{2i\omega T} - Se^{-2i\omega T} &= \frac{1}{2i}\left(e^{2i\omega T} - i\sin 2\omega T\right)\\ &= \frac{1}{2i}\left(e^{2i\omega T} - \frac{1}{2}e^{2i\omega T} + \frac{1}{2}e^{-2i\omega T}\right) = \frac{1}{i}\cos 2\omega T\end{aligned} \tag{7.1}$$

or

$$2\mathrm{R}e^{2i\omega T} = \tfrac{1}{i}\cos 2\omega T \to R = \tfrac{1}{2i}e^{-2i\omega T}\cos 2\omega T$$
$$2Se^{-2i\omega T} = -\tfrac{1}{i}\cos 2\omega T \to S = -\tfrac{1}{2i}e^{2i\omega T}\cos 2\omega T$$

Therefore,

$$a(t) = \mathrm{R}e^{2i\omega t} + Se^{-2i\omega t} + \frac{1}{2} = \frac{1}{2i}\cos 2\omega T\left(e^{-2i\omega T}e^{2i\omega t} - e^{2i\omega T}Se^{-2i\omega t}\right) + \frac{1}{2}$$

$$\begin{aligned}b(t) &= i\mathrm{R}e^{2i\omega t} - iSe^{-2i\omega t} + \frac{i}{2}\sin 2\omega T\\ &= \frac{1}{2}\cos 2\omega T\left(e^{-2i\omega T}e^{2i\omega t} + e^{2i\omega T}Se^{-2i\omega t}\right) + \frac{i}{2}\sin 2\omega T\end{aligned}$$

$$c(t) = b(t) - i\sin 2\omega T = \tfrac{1}{2}\cos 2\omega T\left(e^{-2i\omega T}e^{2i\omega t} + e^{2i\omega T}Se^{-2i\omega t}\right) - \tfrac{i}{2}\sin 2\omega T$$
$$d(t) = 1 - a(t) = \tfrac{1}{2} - \tfrac{1}{2i}\cos 2\omega T\left(e^{-2i\omega T}e^{2i\omega t} - e^{2i\omega T}Se^{-2i\omega t}\right)$$

Consistency checks:

$$Tr\hat{\rho} = a + d = 1 \text{ (true) and } \hat{\rho} = \hat{\rho}^{+} \to b^{*} = c \text{ (true)}$$

Thus,

$$\hat{\rho}(t) = \begin{pmatrix} \frac{1}{2i}\cos 2\omega T\left(e^{2i\omega(t-T)} - e^{-2i\omega(t-T)}\right) + \frac{1}{2} & \frac{1}{2}\cos 2\omega T\left(e^{2i\omega(t-T)} + e^{-2i\omega(t-T)}\right) + \frac{i}{2}\sin 2\omega T \\ \frac{1}{2}\cos 2\omega T\left(e^{2i\omega(t-T)} + e^{-2i\omega(t-T)}\right) - \frac{i}{2}\sin 2\omega T & \frac{1}{2} - \frac{1}{2i}\cos 2\omega T\left(e^{2i\omega(t-T)} - e^{-2i\omega(t-T)}\right) \end{pmatrix}$$

Now

$$\begin{aligned}P(2T) &= Tr(\hat{\rho}(2T)\left|x+\right\rangle\left\langle x+\right|)\\ &= \frac{1}{2}Tr\left(\begin{pmatrix} \cos 2\omega T\sin 2\omega T + \frac{1}{2} & \cos^2 2\omega T + \frac{i}{2}\sin 2\omega T \\ \cos^2 2\omega T - \frac{i}{2}\sin 2\omega T & \frac{1}{2} - \cos 2\omega T\sin 2\omega T \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\right)\\ &= \frac{1}{2}\begin{pmatrix} \cos 2\omega T\sin 2\omega T + \frac{1}{2} + \cos^2 2\omega T + \frac{i}{2}\sin 2\omega T \\ + \cos^2 2\omega T - \frac{i}{2}\sin 2\omega T + \frac{1}{2} - \cos 2\omega T\sin 2\omega T \end{pmatrix}\\ &= \frac{1}{2}\left(1 + 2\cos^2 2\omega T\right)\end{aligned}$$

which agrees with earlier results.

7.7.19 What happens in the Stern-Gerlach box?

An atom with spin = 1/2 passes through a Stern-Gerlach apparatus adjusted so as to transmit atoms that have their spins in the $+z$ direction. The atom spends time T in a magnetic field B in the $x-$direction.

(a) At the end of this time what is the probability that the atom would pass through a Stern-Gerlach selector for spins in the $-z$ direction?

(b) Can this probability be made equal to one, if so, how?

We have

$$\hat{H} = -\vec{\mu} \cdot \vec{B} = \frac{|e| \hbar B}{2mc} \hat{\sigma}_x = \hbar\omega\hat{\sigma}_x \quad , \quad \omega = \frac{|e| B}{2mc}$$

The Schrodinger equation is

$$i\hbar\frac{d}{dt}\begin{pmatrix} a \\ b \end{pmatrix} = \hbar\omega\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \hbar\omega\begin{pmatrix} b \\ a \end{pmatrix} \to i\dot{a} = \omega b \quad , \quad i\dot{b} = \omega a$$

This gives

$$\begin{aligned} &\ddot{a} + \omega^2 a = 0 \to a(t) = \alpha e^{i\omega t} + \beta e^{-i\omega t} \\ &b(t) = \tfrac{i}{\omega}\dot{a} = -\alpha e^{i\omega t} + \beta e^{-i\omega t} \end{aligned}$$

Now,

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

Therefore,

$$\alpha + \beta = 1 \to \alpha = \beta = \frac{1}{2}$$

and

$$\begin{aligned} |\psi(t)\rangle &= \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} e^{i\omega t} + e^{-i\omega t} \\ -e^{i\omega t} + e^{-i\omega t} \end{pmatrix} = \begin{pmatrix} \cos\omega t \\ -i\sin\omega t \end{pmatrix} = \cos\omega t\begin{pmatrix} 1 \\ 0 \end{pmatrix} - i\sin\omega t\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ |\psi(t)\rangle &= \cos\omega t\,|+z\rangle - i\sin\omega t\,|-z\rangle \end{aligned}$$

Now,

$$P(-z;t) = |\langle -z \mid \psi(t)\rangle|^2 = \sin^2\omega t = \frac{1 - \cos 2\omega t}{2}$$

Thus, the probability = 1 if

$$1 - \cos 2\omega t = 2 \to \cos 2\omega t = -1 \to t = \frac{2n+1}{2\omega}\pi = (2n+1)\frac{mc\pi}{|e| B}$$

Alternatively, we have

$$\hat{U} = e^{-i\hat{H}t/\hbar} = e^{-i\omega t\hat{\sigma}_x} = \cos\omega t\hat{I} - i\hat{\sigma}_x\sin\omega t$$

Then

$$
\begin{aligned}
|\psi(t)\rangle &= \hat{U}\,|\psi(0)\rangle = \left(\cos\omega t\hat{I} - i\hat{\sigma}_x \sin\omega t\right)|+z\rangle = \frac{1}{\sqrt{2}}\left(\cos\omega t\hat{I} - i\hat{\sigma}_x \sin\omega t\right)(|+x\rangle + |-x\rangle) \\
&= \frac{1}{\sqrt{2}}\left((\cos\omega t - i\sin\omega t)\,|+x\rangle + (\cos\omega t + i\sin\omega t)\,|-x\rangle\right) \\
&= \frac{1}{\sqrt{2}}\left(e^{-i\omega t}\,|+x\rangle + e^{i\omega t}\,|-x\rangle\right) = \frac{1}{\sqrt{2}}\left(e^{-i\omega t}\frac{1}{\sqrt{2}}(|+z\rangle + |-z\rangle) + e^{i\omega t}\frac{1}{\sqrt{2}}(|+z\rangle - |-z\rangle)\right) \\
&= \cos\omega t\,|+z\rangle - i\sin\omega t\,|-z\rangle
\end{aligned}
$$

as above.

7.7.20 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

$$
\begin{aligned}
|1,1\rangle_x &= \tfrac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \tfrac{1}{2}\,|1,1\rangle + \tfrac{\sqrt{2}}{2}\,|1,0\rangle + \tfrac{1}{2}\,|1,-1\rangle \\
|1,0\rangle_x &= \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \tfrac{1}{\sqrt{2}}\,|1,1\rangle - \tfrac{1}{\sqrt{2}}\,|1,-1\rangle \\
|1,-1\rangle_x &= \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \tfrac{1}{2}\,|1,1\rangle - \tfrac{\sqrt{2}}{2}\,|1,0\rangle + \tfrac{1}{2}\,|1,-1\rangle
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
{}_x\langle 1,1 \mid \psi(0)\rangle &= {}_x\langle 1,1 \mid 1,1\rangle = \tfrac{1}{2} \\
{}_x\langle 1,0 \mid \psi(0)\rangle &= {}_x\langle 1,0 \mid 1,1\rangle = \tfrac{1}{\sqrt{2}} \\
{}_x\langle 1,-1 \mid \psi(0)\rangle &= {}_x\langle 1,-1 \mid 1,1\rangle = \tfrac{1}{2}
\end{aligned}
$$

Now,

$$
\begin{aligned}
\hat{H}\,|1,1\rangle_x &= \omega_0\hat{S}_x\,|1,1\rangle_x = \hbar\omega_0\,|1,1\rangle_x \\
\hat{H}\,|1,0\rangle_x &= \omega_0\hat{S}_x\,|1,0\rangle_x = 0 \\
\hat{H}\,|1,-1\rangle_x &= \omega_0\hat{S}_x\,|1,-1\rangle_x = -\hbar\omega_0\,|1,-1\rangle_x
\end{aligned}
$$

Then,

$$|\psi(t)\rangle = e^{-i\hat{H}t/h}|\psi(0)\rangle = e^{-i\hat{H}t/h}|1,1\rangle = e^{-i\hat{H}t/h}\left(\frac{1}{2}|1,1\rangle_x + \frac{1}{\sqrt{2}}|1,0\rangle_x + \frac{1}{2}|1,-1\rangle_x\right)$$
$$= \frac{1}{2}e^{-i\omega_0 t}|1,1\rangle_x + \frac{1}{\sqrt{2}}|1,0\rangle_x + \frac{1}{2}e^{i\omega_0 t}|1,-1\rangle_x$$

Going back to the $z-$basis we have

$$|\psi(t)\rangle = \frac{1}{2}e^{-i\omega_0 t}\frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} + \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} + \frac{1}{2}e^{i\omega_0 t}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$
$$= \frac{1}{2}\begin{pmatrix} 1+\cos\omega_0 t \\ -\sqrt{2}i\sin\omega_0 t \\ -1+\cos\omega_0 t \end{pmatrix}$$

Finally,

$$P(S_z = -\hbar; t) = |\langle 1,-1 \mid \psi(t)\rangle|^2 = \left|(0,0,1)\,\frac{1}{2}\begin{pmatrix} 1+\cos\omega_0 t \\ -\sqrt{2}i\sin\omega_0 t \\ -1+\cos\omega_0 t \end{pmatrix}\right|^2$$
$$= \left|\frac{1}{2}(-1+\cos\omega_0 t)\right|^2 = \sin^4\frac{\omega_0 t}{2}$$

NOTE: When $\omega_0 t = \pi$, $P(S_z = -\hbar; t = \pi/\omega_0) = 1$. Since $\hat{U}(t) = e^{-i\hat{H}t/h} = e^{-i\omega_0 t\hat{S}_x/h}$, 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.

7.7.21 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

$$|+z'\rangle = \cos\tfrac{\theta}{2}|+z\rangle + \sin\tfrac{\theta}{2}|-z\rangle$$
$$|-z'\rangle = -\sin\tfrac{\theta}{2}|+z\rangle + \cos\tfrac{\theta}{2}|-z\rangle$$
$$|\psi(0)\rangle = |+z\rangle$$

(a) At $t = 0+$, what are the amplitudes for finding the system with spin projections $m' = \pm 1/2$ with respect to the $z'-$axis?

We then have

$$P(+z'; t = 0+) = |\langle +z' \mid \psi(0)\rangle|^2 \, |\langle +z' \mid +z\rangle|^2 = \cos^2 \tfrac{\theta}{2}$$
$$P(-z'; t = 0+) = |\langle -z' \mid \psi(0)\rangle|^2 \, |\langle -z' \mid +z\rangle|^2 = \sin^2 \tfrac{\theta}{2}$$

(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

$$\hat{H} = -\vec{\mu}\cdot\vec{B} = -\mu_0(B_0\hat{\sigma}_z + B_1\hat{\sigma}_x) = -\mu_0 \begin{pmatrix} B_0 & B_1 \\ B_1 & -B_0 \end{pmatrix} = -\mu_0 B \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}$$

where $B = \sqrt{B_0^2 + B_1^2}$. The corresponding eigenvalues/eigenvectors are

$$E_\pm = \mp\mu_0 B = \mp\mu_0\sqrt{B_0^2 + B_1^2}$$
$$|E_\pm\rangle = |\mp z'\rangle$$

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 θ 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

$$\begin{aligned} |\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = \hat{U}(t)|+z\rangle &= e^{-i\mu_0 Bt/\hbar} |-z'\rangle \langle -z' \mid +z\rangle + e^{i\mu_0 Bt/\hbar} |+z'\rangle \langle +z' \mid +z\rangle \\ &= -\sin\frac{\theta}{2} e^{-i\mu_0 Bt/\hbar} |-z'\rangle + \cos\frac{\theta}{2} e^{i\mu_0 Bt/\hbar} |+z'\rangle \end{aligned}$$

and

$$\begin{aligned} P(-z; T) = |\langle -z \mid \psi(T)\rangle|^2 &= \left| -\sin\frac{\theta}{2} e^{-i\mu_0 Bt/\hbar} \langle -z \mid -z'\rangle + \cos\frac{\theta}{2} e^{i\mu_0 Bt/\hbar} \langle -z \mid +z'\rangle \right|^2 \\ &= \left| -\sin\frac{\theta}{2}\cos\frac{\theta}{2} e^{-i\mu_0 Bt/\hbar} + \sin\frac{\theta}{2}\cos\frac{\theta}{2} e^{i\mu_0 Bt/\hbar} \right|^2 = 4\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}\sin^2\frac{\mu_0 Bt}{\hbar} \\ &= \sin^2\theta \sin^2\frac{\mu_0 Bt}{\hbar} \end{aligned}$$

7.7.22 Neutron interferometer

In a classic table-top experiment (neutron interferometer), a monochromatic neutron beam ($\lambda = 1.445 \mathring{A}$) is split by Bragg reflection at point A of an interferometer into two beams which are then recombined (after another reflection) at point D as in Figure 7.1 below:

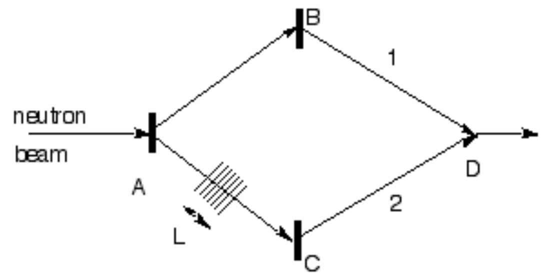


Figure 7.1: Neutron Interferometer Setup

One beam passes through a region of transverse magnetic field of strength B (direction shown by lines)for a distance L. Assume that the two paths from A to D are identical except for the region of magnetic field.

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

$$\psi(t_1) = e^{-i\hat{H}(t_1-t_0)/\hbar}\psi(t_0)$$

where

$$\begin{aligned} t_0 = & \text{ time when neutron enters field region} \\ t_1 = & \text{ time when neutron leaves field region} \end{aligned}$$

We then write

$$\psi(t) = \psi(\vec{r},t)\psi(\vec{s},t) = \text{ (space - part)(spin - part)}$$

which implies that

$$\begin{aligned} \psi(\vec{r},t_1) &= e^{i\left(\frac{\hbar^2}{2m}\nabla^2\right)(t_1-t_0)/\hbar}\psi(\vec{r},t_0) \\ \psi(\vec{s},t_1) &= e^{i\left(\mu\vec{\sigma}\cdot\vec{B}\right)(t_1-t_0)/\hbar}\psi(\vec{s},t_0) \end{aligned}$$

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

$$\psi(\vec{s},t_1) = e^{i\left(\mu\vec{\sigma}\cdot\vec{B}\right)mL\lambda/2\pi\hbar^2}\psi(\vec{s},t_0)$$

where

$$k = \frac{2\pi}{\lambda} = \frac{mv}{\hbar} = \text{ neutron wave number}$$

The intensity of the two beams at D is proportional to

$$\left|\psi_D^{(1)}(\vec{r},t)\psi_D^{(1)}(\vec{s},t) + \psi_D^{(2)}(\vec{r},t)\psi_D^{(2)}(\vec{s},t)\right|^2 \propto \left|\psi_D^{(1)}(\vec{s},t) + \psi_D^{(2)}(\vec{s},t)\right|^2$$

$$= \left|\psi(\vec{s},t_0) + \psi(\vec{s},t_0)e^{i\left(\mu\vec{\sigma}\cdot\vec{B}\right)mL\lambda/2\pi\hbar^2}\right|^2 = \left|\psi(\vec{s},t_0)\right|^2\left|1 + e^{i\left(\mu\vec{\sigma}\cdot\vec{B}/B\right)mL\lambda B/2\pi\hbar^2}\right|^2$$

$$= \left|\psi(\vec{s},t_0)\right|^2\left|1 + \cos\frac{\mu mL\lambda B}{2\pi\hbar^2} + i\vec{\sigma}\cdot\frac{\vec{B}}{B}\sin\frac{\mu mL\lambda B}{2\pi\hbar^2}\right|^2$$

Now,

$$\vec{\sigma}\cdot\frac{\vec{B}}{B} = \pm\sigma$$

depending if $\vec{\sigma}$ is parallel or antiparallel to $\vec{B}$. We then have

$$\begin{aligned} I &= \text{ intensity of interference at } D \\ &= \left|1 + \cos\frac{\mu mL\lambda B}{2\pi\hbar^2} + i\sigma\cdot\sin\frac{\mu mL\lambda B}{2\pi\hbar^2}\right|^2 \\ &= \left(1 + \cos\frac{\mu mL\lambda B}{2\pi\hbar^2}\right)^2 + \sin^2\frac{\mu mL\lambda B}{2\pi\hbar^2} \\ &= 4\cos^2\frac{\mu mL\lambda B}{4\pi\hbar^2} \end{aligned}$$

(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 $-e\hbar/2m_nc$. This calculation was a PRL publication in 1967.

The separation between the maxima is given by

$$\frac{\mu mL\lambda\Delta B}{4\pi\hbar^2} = \pi \to \Delta B = \frac{4\pi^2\hbar^2}{\mu mL\lambda} = \frac{4\pi^2\hbar^2}{\left(\frac{g_ne\hbar}{2mc}\right)mL\lambda} = \frac{8\pi^2\hbar c}{g_neL\lambda}$$

7.7.23 Magnetic Resonance

A particle of spin 1/2 and magnetic moment μ is placed in a magnetic field $\vec{B} = B_0\hat{z} + B_1\hat{x}\cos\omega t - B_1\hat{y}\sin\omega t$, which is often employed in magnetic resonance experiments. Assume that the particle has spin up along the $+z-$axis at $t = 0$ ($m_z = +1/2$). Derive the probability to find the particle with spin down ($m_z = -1/2$) at time $t > 0$.

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

$$\hat{H} = -\gamma\vec{S}\cdot\vec{B} = -\gamma\frac{\hbar}{2}\left(B_0\hat{\sigma}_z + B_1\cos\omega t\hat{\sigma}_x - B_1\sin\omega t\hat{\sigma}_y\right)$$

We first make a transformation to a rotating frame of reference. The equations

$$\begin{aligned} &i\hbar\tfrac{d}{dt}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle \\ &\left|\psi_r(t)\right\rangle = e^{-i\omega t\hat{S}_z/\hbar}\left|\psi(t)\right\rangle \end{aligned}$$

give

$$\begin{aligned} &\hbar\tfrac{d}{dt}e^{i\omega t\hat{S}_z/\hbar}\left|\psi_r(t)\right\rangle = \hat{H}e^{i\omega t\hat{S}_z/\hbar}\left|\psi_r(t)\right\rangle \\ &i\hbar e^{i\omega t\hat{S}_z/\hbar}\tfrac{d}{dt}\left|\psi_r(t)\right\rangle - \omega\hat{S}_z e^{i\omega t\hat{S}_z/\hbar}\left|\psi_r(t)\right\rangle = \hat{H}e^{i\omega t\hat{S}_z/\hbar}\left|\psi_r(t)\right\rangle \\ &i\hbar\tfrac{d}{dt}\left|\psi_r(t)\right\rangle = \omega e^{-i\omega t\hat{S}_z/\hbar}\hat{S}_z e^{i\omega t\hat{S}_z/\hbar}\left|\psi_r(t)\right\rangle + e^{-i\omega t\hat{S}_z/\hbar}\hat{H}e^{i\omega t\hat{S}_z/\hbar}\left|\psi_r(t)\right\rangle \end{aligned}$$

$$\begin{aligned} i\hbar\frac{d}{dt}\left|\psi_r(t)\right\rangle = &\frac{\hbar\omega}{2}\hat{\sigma}_z\left|\psi_r(t)\right\rangle \\ &-\gamma\frac{\hbar}{2}e^{-i\omega t\hat{\sigma}_z/2}\left(B_0\hat{\sigma}_z + B_1\cos\omega t\hat{\sigma}_x - B_1\sin\omega t\hat{\sigma}_y\right)e^{i\omega t\hat{\sigma}_z/2}\left|\psi_r(t)\right\rangle \end{aligned}$$

$$\begin{aligned} i\hbar\frac{d}{dt}\left|\psi_r(t)\right\rangle = &\frac{\hbar\omega}{2}\hat{\sigma}_z\left|\psi_r(t)\right\rangle \\ &-\gamma\frac{\hbar}{2}\left(\begin{array}{l} B_0 e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_z e^{i\omega t\hat{\sigma}_z/2} \\ \quad + B_1\cos\omega t e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_x e^{i\omega t\hat{\sigma}_z/2} - B_1\sin\omega t e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_y e^{i\omega t\hat{\sigma}_z/2} \end{array}\right)\left|\psi_r(t)\right\rangle \end{aligned}$$

$$\begin{aligned} i\hbar\frac{d}{dt}\left|\psi_r(t)\right\rangle = &\frac{\hbar\omega}{2}\hat{\sigma}_z\left|\psi_r(t)\right\rangle \\ &-\gamma\frac{\hbar}{2}\left(B_0\hat{\sigma}_z + B_1\cos\omega t e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_x e^{i\omega t\hat{\sigma}_z/2} - B_1\sin\omega t e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_y e^{i\omega t\hat{\sigma}_z/2}\right)\left|\psi_r(t)\right\rangle \end{aligned}$$

Now

$$e^{\pm i\omega t\hat{\sigma}_z/2} = \cos\frac{\omega t}{2} \pm i\hat{\sigma}_z\sin\frac{\omega t}{2}$$

and therefore,

$$\begin{aligned}
e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_x e^{i\omega t\hat{\sigma}_z/2} &= \left(\cos\frac{\omega t}{2} - i\hat{\sigma}_z\sin\frac{\omega t}{2}\right)\hat{\sigma}_x\left(\cos\frac{\omega t}{2} + i\hat{\sigma}_z\sin\frac{\omega t}{2}\right) \\
&= \cos^2\frac{\omega t}{2}\hat{\sigma}_x + i\cos\frac{\omega t}{2}\sin\frac{\omega t}{2}\left[\hat{\sigma}_x,\hat{\sigma}_z\right] + \sin^2\frac{\omega t}{2}\hat{\sigma}_z\hat{\sigma}_x\hat{\sigma}_z \\
&= \cos^2\frac{\omega t}{2}\hat{\sigma}_x + i\cos\frac{\omega t}{2}\sin\frac{\omega t}{2}\left(-2i\hat{\sigma}_y\right) + \sin^2\frac{\omega t}{2}\left(i\hat{\sigma}_y\hat{\sigma}_z\right) \\
&= \cos^2\frac{\omega t}{2}\hat{\sigma}_x + 2\cos\frac{\omega t}{2}\sin\frac{\omega t}{2}\hat{\sigma}_y - \sin^2\frac{\omega t}{2}\hat{\sigma}_x \\
&= \cos\omega t\hat{\sigma}_x + \sin\omega t\hat{\sigma}_y
\end{aligned}$$

and similarly,

$$e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_y e^{i\omega t\hat{\sigma}_z/2} = -\sin\omega t\hat{\sigma}_x + \cos\omega t\hat{\sigma}_y$$

Therefore,

$$\begin{aligned}
i\hbar\frac{d}{dt}\left|\psi_r(t)\right\rangle &= \frac{\hbar\omega}{2}\hat{\sigma}_z\left|\psi_r(t)\right\rangle \\
&- \gamma\frac{\hbar}{2}\left(\begin{array}{c} B_0\hat{\sigma}_z + B_1\cos\omega t\left(\cos\omega t\hat{\sigma}_x + \sin\omega t\hat{\sigma}_y\right) \\ -B_1\sin\omega t\left(-\sin\omega t\hat{\sigma}_x + \cos\omega t\hat{\sigma}_y\right)\end{array}\right)\left|\psi_r(t)\right\rangle
\end{aligned}$$

$$\begin{aligned}
i\hbar\frac{d}{dt}\left|\psi_r(t)\right\rangle &= \frac{\hbar\omega}{2}\hat{\sigma}_z\left|\psi_r(t)\right\rangle \\
&- \gamma\frac{\hbar}{2}\left(\begin{array}{c} B_0\hat{\sigma}_z + B_1\left(\left(\frac{1}{2}+\frac{1}{2}\cos 2\omega t\right)\hat{\sigma}_x + \frac{1}{2}\sin 2\omega t\hat{\sigma}_y\right) \\ -B_1\sin\omega t\left(-\left(\frac{1}{2}-\frac{1}{2}\cos 2\omega t\right)\hat{\sigma}_x + \frac{1}{2}\sin 2\omega t\hat{\sigma}_y\right)\end{array}\right)\left|\psi_r(t)\right\rangle
\end{aligned}$$

$$\begin{aligned}
i\hbar\frac{d}{dt}\left|\psi_r(t)\right\rangle &= \frac{\hbar\omega}{2}\hat{\sigma}_z\left|\psi_r(t)\right\rangle \\
&- \gamma\frac{\hbar}{2}\left(\begin{array}{c} B_0\hat{\sigma}_z + B_1\left(\frac{\hat{\sigma}_x}{2} + \frac{1}{2}\left(\cos 2\omega t\hat{\sigma}_x + \sin 2\omega t\hat{\sigma}_y\right)\right) \\ -B_1\sin\omega t\left(-\frac{\hat{\sigma}_x}{2} + \frac{1}{2}\left(\cos 2\omega t\hat{\sigma}_x + \sin 2\omega t\hat{\sigma}_y\right)\right)\end{array}\right)\left|\psi_r(t)\right\rangle
\end{aligned}$$

$$i\hbar\frac{d}{dt}\left|\psi_r(t)\right\rangle = \frac{\hbar(\omega-\omega_0)}{2}\hat{\sigma}_z\left|\psi_r(t)\right\rangle - \frac{\hbar\omega_1}{2}\hat{\sigma}_x\left|\psi_r(t)\right\rangle = \frac{\hbar}{2}\left((\omega-\omega_0)\hat{\sigma}_z - \omega_1\hat{\sigma}_x\right)\left|\psi_r(t)\right\rangle$$

where

$$\omega_0 = \gamma B_0 \text{ and } \omega_1 = \gamma B_1$$

We then have

$$i\hbar\frac{d}{dt}\left|\psi_r(t)\right\rangle = \frac{\hbar}{2}\left((\omega-\omega_0)\hat{\sigma}_z - \omega_1\hat{\sigma}_x\right)\left|\psi_r(t)\right\rangle$$

Manipulating this equation we get

$$\frac{d}{dt}\left|\psi_r(t)\right\rangle = -i\frac{\Omega}{2}\hat{\sigma}\left|\psi_r(t)\right\rangle$$

where

$$\hat{\sigma} = \frac{\omega - \omega_0}{\Omega}\hat{\sigma}_z - \frac{\omega_1}{\Omega}\hat{\sigma}_x \text{ and } \Omega^2 = (\omega - \omega_0)^2 + \omega_1^2$$

Since $\hat{\sigma}^2 = \hat{I}$ we can write

$$|\psi_r(t)\rangle = e^{-i\frac{\Omega t}{2}\hat{\sigma}}|\psi_r(0)\rangle$$

and then

$$\begin{aligned} e^{-i\omega t\hat{S}_z/\hbar}|\psi(t)\rangle &= e^{-i\frac{\Omega t}{2}\hat{\sigma}}|\psi(0)\rangle \\ |\psi(t)\rangle &= e^{i\omega t\hat{S}_z/\hbar}e^{-i\frac{\Omega t}{2}\hat{\sigma}}|\psi(0)\rangle \end{aligned}$$

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,

$$\begin{aligned} |\psi(t)\rangle &= e^{i\omega t\hat{S}_z/\hbar}\left(\cos\frac{\Omega t}{2} - i\hat{\sigma}\sin\frac{\Omega t}{2}\right)\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= e^{i\omega t\hat{S}_z/\hbar}\left(\begin{pmatrix} \cos\frac{\Omega t}{2} \\ 0 \end{pmatrix} - i\sin\frac{\Omega t}{2}\left(\frac{\omega - \omega_0}{\Omega}\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{\omega_1}{\Omega}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)\right) \\ &= e^{i\omega t\hat{S}_z/\hbar}\begin{pmatrix} \cos\frac{\Omega t}{2} - i\frac{\omega-\omega_0}{\Omega}\sin\frac{\Omega t}{2} \\ i\frac{\omega_1}{\Omega}\sin\frac{\Omega t}{2} \end{pmatrix} = \begin{pmatrix} \left(\cos\frac{\Omega t}{2} - i\frac{\omega-\omega_0}{\Omega}\sin\frac{\Omega t}{2}\right)e^{i\omega t/2} \\ i\frac{\omega_1}{\Omega}\sin\frac{\Omega t}{2}e^{-i\omega t/2} \end{pmatrix} \end{aligned}$$

Therefore, finally

$$\begin{aligned} |\psi(t)\rangle &= \begin{pmatrix} \left(\cos\frac{\Omega t}{2} - i\frac{\omega-\omega_0}{\Omega}\sin\frac{\Omega t}{2}\right)e^{i\omega t/2} \\ i\frac{\omega_1}{\Omega}\sin\frac{\Omega t}{2}e^{-i\omega t/2} \end{pmatrix} \\ &= \left(\cos\frac{\Omega t}{2} - i\frac{\omega - \omega_0}{\Omega}\sin\frac{\Omega t}{2}\right)e^{i\omega t/2}|z+\rangle + i\frac{\omega_1}{\Omega}\sin\frac{\Omega t}{2}e^{-i\omega t/2}|z-\rangle \end{aligned}$$

and

$$P(z-) = |\langle z- \mid \psi(t)\rangle|^2 = \left|i\frac{\omega_1}{\Omega}\sin\frac{\Omega t}{2}e^{-i\omega t/2}\right|^2 = \left(\frac{\omega_1}{\Omega}\right)^2\sin^2\frac{\Omega t}{2}$$

Alternative solution using differential equations

We have

$$\begin{aligned} \hat{H} &= -\gamma\vec{S}\cdot\vec{B} = -\frac{\hbar}{2}\left(\omega_0\hat{\sigma}_z + \omega_1\cos\omega t\hat{\sigma}_x - \omega_1\sin\omega t\hat{\sigma}_y\right) \\ &= -\frac{\hbar}{2}\omega_0\hat{\sigma}_z - \frac{\hbar}{2}\omega_1\begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \end{aligned}$$

Then

$$\begin{aligned} &i\hbar\tfrac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \\ &i\begin{pmatrix} \dot{a} \\ \dot{b} \end{pmatrix} = -\tfrac{1}{2}\omega_0\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} - \tfrac{1}{2}\omega_1\begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} \end{aligned}$$

so that

$$\begin{aligned}\dot{a} &= \tfrac{i}{2}\omega_0 a + \tfrac{i}{2}\omega_1 e^{i\omega t} b \\ \dot{b} &= -\tfrac{i}{2}\omega_0 b + \tfrac{i}{2}\omega_1 e^{-i\omega t} a\end{aligned}$$

We guess solutions of the form

$$a = \alpha e^{i\omega_0 t/2} \quad , \quad b = \beta e^{-i\omega_0 t/2}$$

which gives

$$\begin{aligned}\dot{\alpha} &= i\tfrac{\omega_1}{2} e^{i(-\omega_0+\omega)t}\beta \\ \dot{\beta} &= i\tfrac{\omega_1}{2} e^{-i(-\omega_0+\omega)t}\alpha\end{aligned}$$

Now assume that

$$\begin{aligned}\alpha &= A_1 e^{i(-\omega_0+\omega+\Omega)t} \\ \beta &= A_2 e^{i\Omega t}\end{aligned}$$

Substitution gives

$$\begin{aligned}&(-\omega_0+\omega+\Omega)A_1 - \tfrac{\omega_1}{2}A_2 = 0 \\ &-\tfrac{\omega_1}{2}A_1 + \Omega A_2 = 0\end{aligned}$$

These homogeneous equations have a non-trivial solution only if

$$\begin{vmatrix} -\omega_0+\omega+\Omega & -\frac{\omega_1}{2} \\ -\frac{\omega_1}{2} & \Omega \end{vmatrix} = 0 = \Omega\left(-\omega_0+\omega+\Omega\right) - \frac{\omega_1^2}{4} = 0$$

so that

$$\Omega_\pm = \frac{\omega-\omega_0}{2} \pm \frac{1}{2}\sqrt{\left(\omega-\omega_0\right)^2+\omega_1^2} = \frac{\omega-\omega_0}{2} \pm \frac{\Omega}{2}$$

where

$$\Omega = \sqrt{\left(\omega-\omega_0\right)^2+\omega_1^2}$$

Therefore, the most general solutions are

$$\begin{aligned}\beta &= A_{2+}e^{i\Omega_+ t} + A_{2-}e^{i\Omega_- t} \\ \alpha &= -\tfrac{i2}{\omega_1}e^{i(-\omega_0+\omega)t}\dot{\beta} = \tfrac{2}{\omega_1}e^{i(-\omega_0+\omega)t}\left(\Omega_+ A_{2+}e^{i\Omega_+ t} + \Omega_- A_{2-}e^{i\Omega_- t}\right)\end{aligned}$$

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,

$$\begin{aligned}0 &= A_{2+} + A_{2-} \\ 1 &= \tfrac{2}{\omega_1}\left(\Omega_+ A_{2+} + \Omega_- A_{2-}\right)\end{aligned}$$

or

$$A_{2+} = -A_{2-} = \frac{1}{2}\frac{\omega_1}{\Omega_+ - \Omega_-} = \frac{\omega_1}{2\Omega}$$

so that

$$\begin{aligned} b(t) = \beta(t)e^{-i\omega_0 t/2} &= e^{-i\omega_0 t/2} A_{2+}\left(e^{i\Omega_+ t} - e^{i\Omega_- t}\right) \\ &= e^{-i\omega_0 t/2} e^{i\frac{\omega-\omega_0}{2}t} A_{2+}\left(e^{i\Omega t/2} - e^{-i\Omega t/2}\right) \\ &= e^{-i\omega_0 t/2} e^{i\frac{\omega-\omega_0}{2}t} \frac{\omega_1}{\Omega}\left(i\sin\frac{\Omega t}{2}\right) \end{aligned}$$

Finally,

$$P = |b(t)|^2 = \left|e^{-i\omega_0 t/2} e^{i\frac{\omega-\omega_0}{2}t} \frac{\omega_1}{\Omega}\left(i\sin\frac{\Omega t}{2}\right)\right|^2 = \frac{\omega_1^2}{\Omega^2}\sin^2\frac{\Omega t}{2}$$

as in the earlier discussion.

7.7.24 More addition of angular momentum

Consider a system of two particles with $j_1 = 2$ and $j_2 = 1$. Determine the $|j, m, j_1, j_2\rangle$ states listed below in the $|j_1, m_1, j_2, m_2\rangle$ basis.

$$|3,3,j_1,j_2\rangle \ , \ |3,2,j_1,j_2\rangle \ , \ |3,1,j_1,j_2\rangle \ , \ |2,2,j_1,j_2\rangle \ , \ |2,1,j_1,j_2\rangle \ , \ |1,1,j_1,j_2\rangle$$

We have $2 \otimes 1 = 1 \oplus 2 \oplus 3$. Now in the $|m_1, m_2\rangle$ basis

$$j_1 = 2 \rightarrow m_1 = \pm 2, \pm 1, 0 \rightarrow 5 \text{ states and } j_2 = 1 \rightarrow m_2 = \pm 1, 0 \rightarrow 3 \text{ states}$$

so that we have a total of $5 \times 3 = 15$ states.

Similarly, in the $|J, M\rangle$ basis

$$\begin{aligned} &J = 3 \rightarrow M = \pm 3, \pm 2, \pm 1, 0 \rightarrow 7 \text{ states} \\ &J = 2 \rightarrow M = \pm 2, \pm 1, 0 \rightarrow 5 \text{ states} \\ &J = 1 \rightarrow M = \pm 1, 0 \rightarrow 3 \text{ states} \end{aligned}$$

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 $|m_1, m_2\rangle = |m_1, m_2\rangle_m$ states.

Remember

$$J_- |j, m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\, |j, m-1\rangle$$

The *highest* $|J, M\rangle$ is $|3,3\rangle = |2,1\rangle_m$. Therefore,

$$\begin{aligned} &J_- |3,3\rangle = \sqrt{6}\hbar\, |3,2\rangle = (J_{1-} + J_{2-})\, |2,1\rangle_m = 2\hbar\, |1,1\rangle_m + \sqrt{2}\hbar\, |2,0\rangle_m \\ &\rightarrow |3,2\rangle = \sqrt{\tfrac{2}{3}}\, |1,1\rangle_m + \sqrt{\tfrac{1}{3}}\, |2,0\rangle_m \end{aligned}$$

and

$$J_- |3,2\rangle = \sqrt{10}\hbar |3,1\rangle = (J_{1-} + J_{2-}) \left(\sqrt{\frac{2}{3}} |1,1\rangle_m + \sqrt{\frac{1}{3}} |2,0\rangle_m \right)$$

$$= \sqrt{\frac{2}{3}} \sqrt{6}\hbar |0,1\rangle_m + \sqrt{\frac{1}{3}} 2\hbar |1,0\rangle_m + \sqrt{\frac{2}{3}} \sqrt{2}\hbar |1,0\rangle_m + \sqrt{\frac{1}{3}} \sqrt{2}\hbar |2,-1\rangle_m$$

$$\to |3,1\rangle = \sqrt{\frac{8}{15}} |1,0\rangle_m + \sqrt{\frac{2}{5}} |0,1\rangle_m + \sqrt{\frac{1}{15}} |2,-1\rangle_m$$

Now

$$|2,2\rangle = a |1,1\rangle_m + b |2,0\rangle_m \quad , \quad a^2 + b^2 = 1$$

and

$$\langle 3,2 \mid 2,2\rangle = 0 = \sqrt{\frac{2}{3}} a + \sqrt{\frac{1}{3}} b$$

which gives

$$b = -\sqrt{2} a \to a = \sqrt{\frac{1}{3}} \to b = -\sqrt{\frac{2}{3}}$$

so that

$$|2,2\rangle = \sqrt{\frac{1}{3}} |1,1\rangle_m - \sqrt{\frac{2}{3}} |2,0\rangle_m$$

Then

$$J_- |2,2\rangle = 2\hbar |2,1\rangle = (J_{1-} + J_{2-}) \left(\sqrt{\frac{1}{3}} |1,1\rangle_m - \sqrt{\frac{2}{3}} |2,0\rangle_m \right)$$

$$= \sqrt{\frac{1}{3}} \sqrt{6}\hbar |0,1\rangle_m - \sqrt{\frac{2}{3}} 2\hbar |1,0\rangle_m + \sqrt{\frac{1}{3}} \sqrt{2}\hbar |1,0\rangle_m - \sqrt{\frac{2}{3}} \sqrt{2}\hbar |2,-1\rangle_m$$

$$\to |2,1\rangle = \sqrt{\frac{1}{2}} |0,1\rangle_m - \sqrt{\frac{1}{6}} |1,0\rangle_m - \sqrt{\frac{1}{3}} |2,-1\rangle_m$$

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

$$\langle 2,1 \mid 1,1\rangle = 0 = \sqrt{\tfrac{1}{2}} a - \sqrt{\tfrac{1}{6}} b - \sqrt{\tfrac{1}{3}} c$$
$$\langle 3,1 \mid 1,1\rangle = 0 = \sqrt{\tfrac{2}{5}} a + \sqrt{\tfrac{8}{15}} b + \sqrt{\tfrac{1}{15}} c$$

so that

$$c = \sqrt{6} a \quad , \quad b = -\sqrt{3} a$$
$$a = \sqrt{\tfrac{1}{10}} \to b = -\sqrt{\tfrac{3}{10}} \quad , \quad c = \sqrt{\tfrac{3}{5}}$$

and

$$|1,1\rangle = \sqrt{\frac{1}{10}} |0,1\rangle_m - \sqrt{\frac{3}{10}} |1,0\rangle_m + \sqrt{\frac{3}{5}} |2,-1\rangle_m$$

7.7.25 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 $|2, 2\rangle = \left|\frac{3}{2}, \frac{3}{2}\right\rangle^a \left|\frac{1}{2}, \frac{1}{2}\right\rangle^b$. 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

$$J_- |2,2\rangle = 2|2,1\rangle = \left(J_-^a + J_-^b\right) \left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b = \sqrt{3} \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b + \left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b$$
$$\rightarrow |2,1\rangle = \tfrac{\sqrt{3}}{2} \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b + \tfrac{1}{2} \left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b$$

and

$$J_- |2,1\rangle = \sqrt{6}\,|2,0\rangle = \left(J_-^a + J_-^b\right) \left(\frac{\sqrt{3}}{2} \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b + \frac{1}{2} \left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b \right)$$
$$= \frac{\sqrt{3}}{2} 2 \left|\tfrac{3}{2}, -\tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b + \frac{\sqrt{3}}{2} \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b + \frac{\sqrt{3}}{2} \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b$$
$$\rightarrow |2,0\rangle = \frac{1}{\sqrt{2}} \left|\tfrac{3}{2}, -\tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b + \frac{1}{\sqrt{2}} \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b$$

Similarly,

$$|2,-1\rangle = \frac{\sqrt{3}}{2} \left|\tfrac{3}{2}, -\tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b + \frac{1}{2} \left|\tfrac{3}{2}, -\tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b$$

and

$$|2,-2\rangle = \left|\tfrac{3}{2}, -\tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b$$

To find the $|1, m\rangle$ states we start with $|1, 1\rangle$ which must be a linear combination

$$|1,1\rangle = a \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b + b \left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b$$

with

$$a^2 + b^2 = 1 \text{ and } \langle 1,1 \mid 2,1\rangle = 0 = \frac{\sqrt{3}}{2} a + \frac{1}{2} b$$

or

$$b = -\sqrt{3} a \rightarrow 4a^2 = 1 \rightarrow a = \frac{1}{2} \rightarrow b = -\frac{\sqrt{3}}{2}$$

so that

$$|1,1\rangle = \frac{1}{2} \left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle^b - \frac{\sqrt{3}}{2} \left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle^b$$

Using the same procedure as above we find

$$|1,0\rangle = \frac{1}{\sqrt{2}}\left|\tfrac{3}{2},\tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle^b - \frac{1}{\sqrt{2}}\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle^b$$
$$|1,-1\rangle = -\frac{\sqrt{3}}{2}\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle^a \left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle^b + \frac{1}{2}\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle^a \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle^b$$

All states are automatically normalized to unity and all orthogonality relations are satisfied.

7.7.26 Spin$-1/2$ and Density Matrices

Let us consider the application of the density matrix formalism to the problem of a spin$-1/2$ particle in a static external magnetic field. In general, a particle with spin may carry a magnetic moment, oriented along the spin direction (by symmetry). For spin$-1/2$, we have that the magnetic moment (operator) is thus of the form:

$$\hat{\mu}_i = \frac{1}{2}\gamma\hat{\sigma}_i$$

where the $\hat{\sigma}_i$ are the Pauli matrices and γ is a constant giving the strength of the moment, called the gyromagnetic ratio. The term in the Hamiltonian for such a magnetic moment in an external magnetic field, $\vec{B}$ is just:

$$\hat{H} = -\vec{\mu}\cdot\vec{B}$$

The spin$-1/2$ particle has a spin orientation or *polarization* given by

$$\vec{P} = \langle\vec{\sigma}\rangle$$

Let us investigate the motion of the polarization vector in the external field. Recall that the expectation value of an operator may be computed from the density matrix according to

$$\left\langle \hat{A} \right\rangle = Tr\left(\hat{\rho}\hat{A}\right)$$

In addition the time evolution of the density matrix is given by

$$i\frac{\partial\hat{\rho}}{\partial t} = \left[\hat{H}(t), \hat{\rho}(t)\right]$$

Determine the time evolution $d\vec{P}/dt$ of the polarization vector. Do not make any assumption concerning the purity of the state. Discuss the physics involved in your results.

Let us consider the i^{th} component of the polarization

$$\begin{aligned}
i\frac{dP_i}{dt} &= i\frac{d\left\langle \sigma_i \right\rangle}{dt} = i\frac{d}{dt}Tr(\rho\sigma_i) = iTr(\frac{\partial \rho}{\partial t}\sigma_i) \\
&= Tr(\left[\hat{H},\hat{\rho}\right]\sigma_i) = Tr(\hat{H}\hat{\rho}\sigma_i - \hat{\rho}\hat{H}\sigma_i) \\
&= Tr(\sigma_i\hat{H}\hat{\rho} - \hat{H}\sigma_i\hat{\rho}) = Tr(\left[\sigma_i,\hat{H}\right]\hat{\rho}) \\
&= -Tr(\left[\sigma_i,\vec{\mu}\cdot\vec{B}\right]\hat{\rho}) = -\frac{1}{2}\gamma Tr\left(\left[\sigma_i,\sum_{j=1}^{3}\hat{\sigma}_j B_j\right]\hat{\rho}\right) \\
&= -\frac{1}{2}\gamma\sum_{j=1}^{3}B_j Tr(\left[\hat{\sigma}_i,\hat{\sigma}_j\right]\hat{\rho})
\end{aligned}$$

To proceed further, we need the density matrix for a state with polarization $\vec{P}$. Since $r\hat{h}o$ is hermitian, it must be of the form

$$\hat{\rho} = a(\hat{I} + \vec{b}\cdot\vec{\sigma})$$

that is, $\left\{\hat{I},\vec{\sigma}\right\}$ are a basis set for all 2×2 matrices. Buts its trace must be one, so that

$$Tr\hat{\rho} = 1 = a(Tr\hat{I} + Tr(\vec{b}\cdot\vec{\sigma})) = a(2+0) \Rightarrow a = 1/2$$

Finally, to get the right polarization vector, we must have

$$\begin{aligned}
Tr\left(\hat{\rho}\vec{\sigma}\right) = \left\langle\vec{\sigma}\right\rangle = \vec{P} &= a(Tr\vec{\sigma} + Tr\left((\vec{b}\cdot\vec{\sigma})\vec{\sigma}\right)) \\
&= \frac{1}{2}(0 + Tr\left((\vec{b}\cdot\vec{\sigma})\vec{\sigma}\right) = \frac{1}{2}Tr\left((\vec{b}\cdot\vec{\sigma})\vec{\sigma}\right)
\end{aligned}$$

Now

$$\vec{b}\cdot\left((\vec{b}\cdot\vec{\sigma})\vec{\sigma}\right) = (\vec{b}\cdot\vec{\sigma})(\vec{b}\cdot\vec{\sigma}) = \vec{b}\cdot\vec{b} + i\vec{\sigma}\cdot\vec{b}\times\vec{b} = \vec{b}\cdot\vec{b}$$

or

$$(\vec{b}\cdot\vec{\sigma})\vec{\sigma} = \vec{b}$$

so that

$$\vec{P} = Tr\left(\hat{\rho}\vec{\sigma}\right) = \frac{1}{2}Tr\left((\vec{b}\cdot\vec{\sigma})\vec{\sigma}\right) = \frac{\vec{b}}{2}Tr\hat{I} = \vec{b}$$

Thus, we have

$$i\frac{dP_i}{dt} = -\frac{1}{4}\gamma\sum_{j=1}^{3}B_j\left\{Tr(\left[\hat{\sigma}_i,\hat{\sigma}_j\right]) + \sum_{k=1}^{3}P_k Tr(\left[\hat{\sigma}_i,\hat{\sigma}_j\right]\hat{\sigma}_k)\right\}$$

Now $\left[\hat{\sigma}_i,\hat{\sigma}_j\right] = 2i\varepsilon_{ijk}\hat{\sigma}_k$, which is traceless. Further,

$$Tr(\left[\hat{\sigma}_i,\hat{\sigma}_j\right]\hat{\sigma}_k) = 2i\varepsilon_{ijk}Tr(\hat{\sigma}_k\hat{\sigma}_k) = 4i\varepsilon_{ijk}$$

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 $\vec{B}$.

7.7.27 System of N Spin$-1/2$ Particle

Let us consider a system of N spin$-1/2$ particles per unit volume in thermal equilibrium, in an external magnetic field $\vec{B}$. In thermal equilibrium the canonical distribution applies and we have the density operator given by:

$$\hat{\rho} = \frac{e^{-\hat{H}t}}{Z}$$

where Z is the partition function given by

$$Z = Tr\left(e^{-\hat{H}t}\right)$$

Such a system of particles will tend to orient along the magnetic field, resulting in a bulk magnetization (having units of magnetic moment per unit volume), $\vec{M}$.

(a) Give an expression for this magnetization $\vec{M} = N\gamma\langle\vec{\sigma}/2\rangle$(don't 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

$$M_z = N\frac{1}{2}\gamma\langle\sigma_z\rangle = N\gamma\frac{1}{2Z}Tr\left(e^{-H/T}\sigma_z\right)$$

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.,

$$e^{-H/T} \approx 1 - \frac{H}{T} = 1 + \frac{\gamma B_z}{2T}$$

Thus,

$$M_z = N\gamma\frac{1}{2Z}Tr\left(\left(1 + \frac{\gamma B_z}{2T}\right)\sigma_z\right) = N\gamma^2 B_z \frac{1}{2ZT}$$

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.

7.7.28 In a coulomb field

An electron in the Coulomb field of the proton is in the state

$$|\psi\rangle = \frac{4}{5}|1,0,0\rangle + \frac{3i}{5}|2,1,1\rangle$$

where the $|n,\ell,m\rangle$ are the standard energy eigenstates of hydrogen.

(a) What is $\langle E\rangle$ for this state? What are $\left\langle \hat{L}^2\right\rangle$, $\left\langle \hat{L}_x\right\rangle$ and $\left\langle \hat{L}_x\right\rangle$?

$$\langle E\rangle = E_1P(E_1) + E_2P(E_2) = \left(\tfrac{4}{5}\right)^2\left(-\tfrac{1}{2}\mu c^2\alpha^2\right) + \left(\tfrac{3}{5}\right)^2\left(-\tfrac{1}{8}\mu c^2\alpha^2\right) = -\tfrac{73}{200}\mu c^2\alpha^2$$
$$\left\langle L^2\right\rangle = (L^2)_1P((L^2)_1) + (L^2)_2P((L^2)_2) = \left(\tfrac{4}{5}\right)^2(0) + \left(\tfrac{3}{5}\right)^2\left(2\hbar^2\right) = \tfrac{18}{25}\hbar^2$$
$$\langle L_z\rangle = (L_z)_1P((L_z)_1) + (L_z)_2P((L_z)_2) = \left(\tfrac{4}{5}\right)^2(0) + \left(\tfrac{3}{5}\right)^2(\hbar) = \tfrac{9}{25}\hbar$$

(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.

7.7.29 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,

$$-\frac{e^2}{r_+} = E_1 = -\frac{1}{2}\mu c^2\alpha^2 \rightarrow r_+ = \frac{2e^2}{\mu c^2\alpha^2} = 2\frac{\hbar}{\mu c\alpha} = 2a_0$$

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

$$\begin{aligned} P(r \geq r_+) &= \int_{2a_0}^{\infty} R_{10}^2(r) r^2 dr = \frac{4}{a_0^3}\int_{2a_0}^{\infty} e^{-2r/a_0} r^2 dr \\ &= \frac{4}{a_0^3}\left[\frac{r^2 e^{-2r/a_0}}{(-2/a_0)} - \frac{2}{(-2/a_0)}\frac{e^{-2r/a_0}}{(-2/a_0)^2}\left(-\frac{2r}{a_0} - 1\right)\right]_{r=2a_0}^{r=\infty} \\ &= \frac{4e^{-4}}{a_0^3}\left[2a_0^3 + \frac{5}{4}a_0^3\right] = 13e^{-4} = 0.24 \end{aligned}$$

(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

$$\begin{aligned} |initial\rangle &= |1,0,0;Z=1\rangle \\ |final\rangle &= |1,0,0;Z=2\rangle \end{aligned}$$

Therefore,

$$\begin{aligned} \langle final \mid initial\rangle &= \int d^3r \,\langle final \mid \vec{r}\rangle\,\langle \vec{r} \mid initial\rangle = \int_0^{\infty} R_{10}^{Z=2} R_{10}^{Z=1} r^2 dr \\ &= \frac{4}{a_0^3} 2^{3/2}\int_0^{\infty} e^{-3r/a_0} r^2 dr = 8\frac{2^{3/2}}{3^3} \end{aligned}$$

Therefore,

$$P(remain) = |\langle final \mid initial\rangle|^2 = \left|8\frac{2^{3/2}}{3^3}\right|^2 = \frac{64\cdot 8}{(27)^2} = 0.70$$

7.7.30 What happens?

At the time $t = 0$ the wave function for the hydrogen atom is

$$\psi(\vec{r}, 0) = \frac{1}{\sqrt{10}} \left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21-1} \right)$$

where the subscripts are the values of the quantum numbers $(n\ell m)$. We ignore spin and any radiative transitions.

(a) What is the expectation value of the energy in this state?

$$\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle = \sum_n E_n P(E_n) = \frac{1}{10} (4E_1 + E_2 + 2E_2 + 3E_2)$$
$$= \frac{1}{5} (2E_1 + 3E_2) = 0.55E_1 = -0.55(13.6) = -7.47\, eV$$

(b) What is the probability of finding the system with $\ell = 1$, $m = +1$ as a function of time?

$$P_{11}(t) = |\langle 2,1,1 \mid \psi(t) \rangle|^2 = \left| \langle 2,1,1 | \, e^{-i\hat{H}t/\hbar} \, | \psi(0) \rangle \right|^2$$
$$= \left| \langle 2,1,1 | \left(\frac{1}{\sqrt{10}} \left(\begin{array}{c} 2e^{-iE_1 t/\hbar} |1,0,0\rangle + e^{-iE_2 t/\hbar} |2,1,0\rangle \\ +\sqrt{2} e^{-iE_2 t/\hbar} |2,1,1\rangle + \sqrt{3} e^{-iE_2 t/\hbar} |2,1,-1\rangle \end{array} \right) \right) \right|^2$$
$$= \frac{1}{5}$$

(c) What is the probability of finding an electron within $10^{-10}\, cm$ of the proton (at time $t = 0$)? A good approximate result is acceptable.

Let $\alpha = 10^{-10} cm$. Then we have

$$P(r < \alpha; t = 0) = \int_0^\alpha \psi^*(0)\psi(0) r^2 dr d\Omega = \frac{1}{10} \int_0^\alpha \left(4R_{10}^2 + 6R_{21}^2 \right) r^2 dr$$

where

$$R_{10}^2 = \frac{4}{a^3} e^{-2r/a} \quad , \quad R_{21}^2 = \frac{r^2}{24a^5} e^{-r/2a} \quad , \quad a = a_0 = 5.29 \times 10^{-9} cm$$

Since $r \leq \alpha << a$ we can make approximations

$$R_{10}^2 = \frac{4}{a^3} \left(1 - \frac{2r}{a} \right) \quad , \quad R_{21}^2 = \frac{r^2}{24a^5} \left(1 - \frac{r}{2a} \right)$$

Therefore,

$$P(r < \alpha; t=0) = \frac{4}{10}\frac{4}{a^3}\int_0^\alpha \left(1 - \frac{2r}{a}\right) r^2 dr + \frac{6}{10}\frac{1}{24a^5}\int_0^\alpha \left(1 - \frac{r}{2a}\right) r^4 dr$$
$$= \frac{4}{10}\left[\frac{4}{3}\left(\frac{\alpha}{a}\right)^3 - 2\left(\frac{\alpha}{a}\right)^4\right] + \frac{6}{10}\left[\frac{1}{120}\left(\frac{\alpha}{a}\right)^5 - \frac{1}{288}\left(\frac{\alpha}{a}\right)^6\right]$$
$$\approx \frac{8}{15}\left(\frac{\alpha}{a}\right)^3 = 3.6 \times 10^{-6}$$

(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

$$\hat{L}_x |\psi\rangle = C_0 \hat{L}_x |2,1,0\rangle + C_+ \hat{L}_x |2,1,1\rangle + C_- \hat{L}_x |2,1,-1\rangle$$
$$= |\psi\rangle = C_0 |2,1,0\rangle + C_+ |2,1,1\rangle + C_- |2,1,-1\rangle$$

$$\rightarrow \frac{1}{2}\left(\sqrt{2}C_0 |2,1,1\rangle + \sqrt{2}(C_+ + C_-)|2,1,0\rangle + \sqrt{2}C_0 |2,1,-1\rangle\right)$$
$$= C_0 |2,1,0\rangle + C_+ |2,1,1\rangle + C_- |2,1,-1\rangle$$

$$\rightarrow C_+ = C_- = \frac{C_0}{\sqrt{2}} \rightarrow |\psi\rangle = \frac{1}{2}C_0\left(2|2,1,0\rangle + \sqrt{2}|2,1,1\rangle + \sqrt{2}|2,1,-1\rangle\right)$$

Normalizing gives $C_0 = 1/\sqrt{2}$ so that

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

7.7.31 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

$$\psi_{n_1 n_2 n_3}(x_1, x_2, x_3) = e^{-\frac{1}{2}\frac{m\omega_1}{\hbar}x_1^2} H_{n_1}\left(\sqrt{\frac{m\omega_1}{\hbar}}x_1\right) e^{-\frac{1}{2}\frac{m\omega_2}{\hbar}x_2^2} H_{n_2}\left(\sqrt{\frac{m\omega_2}{\hbar}}x_2\right) \times e^{-\frac{1}{2}\frac{m\omega_3}{\hbar}x_3^2} H_{n_3}\left(\sqrt{\frac{m\omega_3}{\hbar}}x_3\right)$$

with

$$\omega_0 = \omega_1 = \omega_2 = \omega\sqrt{1-\tau} \quad , \quad \omega_3 = \omega\sqrt{1+\tau}$$

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 τ, the variation of the energy and the degree of degeneracy of the ground state and the first two excited states.

For generic values of τ, 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 $n_1 = 0, 1, 2, ..., n - n_3$ 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,

$$E(1,0) = 2\hbar\omega\sqrt{1-\tau} + \tfrac{1}{2}\hbar\omega\sqrt{1+\tau}$$
$$E(1,1) = \hbar\omega\sqrt{1-\tau} + \tfrac{3}{2}\hbar\omega\sqrt{1+\tau}$$

$E(1,0)$ 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 τ, 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 τ 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

$$E(0,0) = 2\hbar\omega\sqrt{1-\tau}$$
$$E(1,0) = 3\hbar\omega\sqrt{1-\tau}$$
$$E(1,1) = 4\hbar\omega\sqrt{1-\tau}$$

so the levels remain separated. However, for $n = 2$, we have the levels

$$E(2,0) = 4\hbar\omega\sqrt{1-\tau}$$
$$E(2,1) = 5\hbar\omega\sqrt{1-\tau}$$
$$E(2,2) = 6\hbar\omega\sqrt{1-\tau}$$

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 τ.

Evidently, similar *coincidental* degeneracies occur whenever τ is such that $\sqrt{1+\tau} = N\sqrt{1-\tau}$, with N a positive integer.

7.7.32 Exponential potential

Two particles, each of mass M, are attracted to each other by a potential

$$V(r) = -\left(\frac{g^2}{d}\right)e^{-r/d}$$

where $d = \hbar/mc$ with $mc^2 = 140\,MeV$ and $Mc^2 = 940\,MeV$.

(a) Show that for $\ell = 0$ the radial Schrodinger equation for this system can be reduced to Bessel's differential equation

$$\frac{d^2 J_\rho(x)}{dx^2} + \frac{1}{x}\frac{dJ_\rho(x)}{dx} + \left(1 - \frac{\rho^2}{x^2}\right)J_\rho(x) = 0$$

by means of the change of variable $x = \alpha e^{-\beta r}$ for a suitable choice of α and β.

When $\ell = 0$, the radial wave function $R(r) = \chi(r)/r$ satisfies the equation

$$\frac{d^2\chi}{dr^2} + \frac{M}{\hbar^2}\left(E + \frac{g^2}{d}e^{-r/d}\right)\chi = 0$$

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

$$\frac{d}{dr} = \frac{dx}{dr}\frac{d}{dx} = -\beta\alpha e^{-\beta r}\frac{d}{dx} = -\beta x\frac{d}{dx}$$
$$\frac{d^2}{dr^2} = \frac{dx}{dr}\frac{d}{dx}\left(\frac{d}{dr}\right) = \frac{dx}{dr}\frac{d}{dx}\left(-\beta x\frac{d}{dx}\right) = -\beta x\left(-\beta\frac{d}{dx} - \beta x\frac{d^2}{dx^2}\right)$$

Therefore,

$$-\beta x\left(-\beta\frac{d}{dx}-\beta x\frac{d^2}{dx^2}\right)J(x)+\frac{M}{\hbar^2}\left(E+\frac{g^2}{d}\left(\frac{x}{\alpha}\right)^{1/d\beta}\right)J(x)=0$$
$$\frac{d^2J}{dx^2}+\frac{1}{x}\frac{dJ}{dx}+\frac{M}{\beta\hbar^2x^2}\left(E+\frac{g^2}{d}\left(\frac{x}{\alpha}\right)^{1/d\beta}\right)J=0$$

We now choose

$$\alpha=\frac{2g}{\hbar}\sqrt{Md} \quad , \quad \beta=\frac{1}{2d} \quad , \quad \rho^2=\frac{4d^2M\left|E\right|}{\hbar^2}$$

so that the equation becomes Bessel's equation of order ρ

$$\frac{d^2J_\rho(x)}{dx^2}+\frac{1}{x}\frac{dJ_\rho(x)}{dx}+\left(1-\frac{\rho^2}{x^2}\right)J_\rho(x)=0$$

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

$$\lim_{r\to\infty}R(r)\to 0\to J_\rho \text{ remains finite or } \rho\geq 0$$

$R(r)$ must also be finite at $r=0$, which means that $\chi(0)=J_\rho(\alpha)=0$. This equation has an infinite number of real roots.

For

$$E=2.2\,MeV, \quad \rho=\frac{2d}{\hbar}\sqrt{M\left|E\right|}=\frac{2}{mc^2}\sqrt{Mc^2\left|E\right|}=\frac{2}{140}\sqrt{940\cdot 2.2}\approx 0.65$$

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 OCTAVE code below).

```
OCTAVE code:

n=0.05*(0:40);x=0.05*(0:160);
nx=length(x);nn=length(n);
ox=ones(1,nn);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');
```

```
clabel(C,h);
hold on
plot([0.65,0.65],[0.0,8.0],'--k')
xlabel('\rho','FontSize',20)
ylabel('\alpha','FontSize',20)
title('J_\rho(\alpha) in \rho-\alpha plane','FontSize',20)
hold off
```

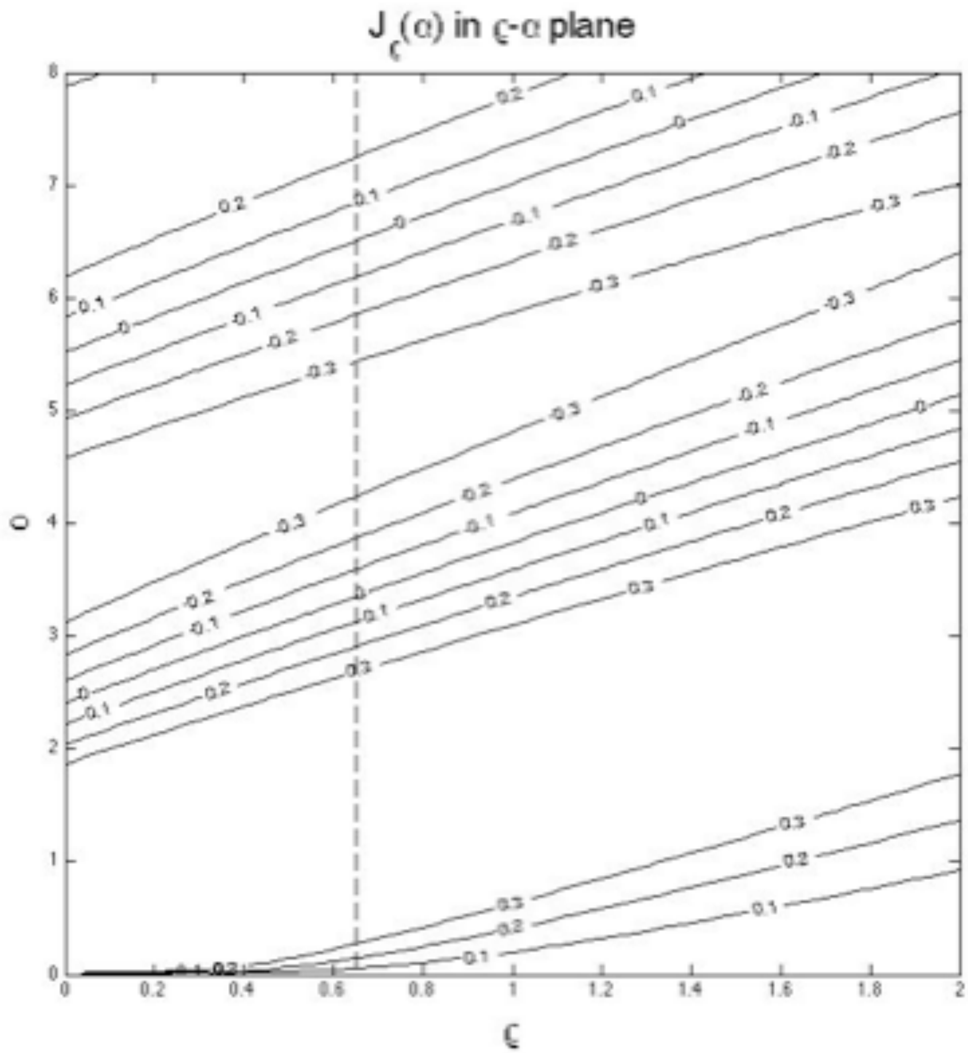


Figure 7.2: $J_\rho(\alpha)$ contours in the $\alpha - \rho$ plane

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

$$\frac{g^2}{\hbar c} = \frac{\hbar\alpha^2}{4Mcd} = \frac{\hbar mc^2\alpha^2}{4Mc^2} \approx 0.41 \text{ (dimensionless)}$$

(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 α for two $\ell = 0$ bound states is 6.6, for which

$$\frac{g^2}{\hbar c} = \frac{\hbar mc^2\alpha^2}{4Mc^2} \approx 1.62$$

7.7.33 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 7.3 below:

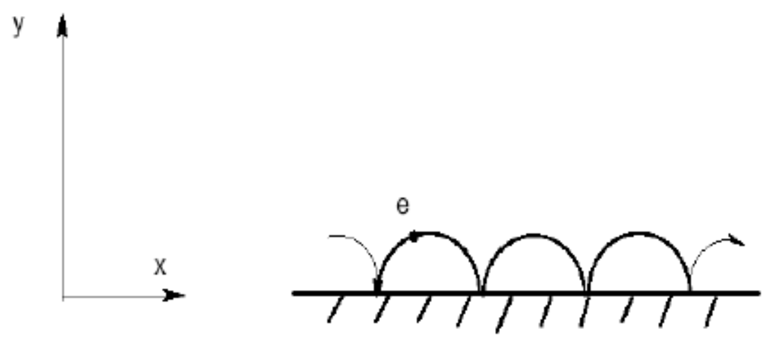


Figure 7.3: Bouncing electrons

(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 Schrodinger 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

$$\begin{aligned}
&\psi(x,y,z) = \psi_n(y)\varphi_x(x)\varphi_z(z) \\
&-\tfrac{\hbar^2}{2m}\tfrac{d^2\psi_n(y)}{dy^2} - \tfrac{e^2}{4y}\psi_n(y) = E_y\psi_n(y) \\
&-\tfrac{\hbar^2}{2m}\tfrac{d^2\varphi_x(x)}{dx^2} = \tfrac{p_x^2}{2m}\varphi_x(x) \quad , \quad -\tfrac{\hbar^2}{2m}\tfrac{d^2\varphi_z(z)}{dz^2} = \tfrac{p_z^2}{2m}\varphi_z(z) \\
&E = \tfrac{p_x^2}{2m} + \tfrac{p_z^2}{2m} + E_y
\end{aligned}$$

Note that since

$$V(\vec{r}) = -\frac{e^2}{4y}$$

depends only on y, p_x and p_z are constant of the motion. Therefore,

$$\varphi_x(x) = e^{ip_x x/\hbar} \quad , \quad \varphi_z(z) = e^{ip_z z/\hbar}$$

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

$$\psi(x,y,z) = 0 \quad for \quad y \leq 0$$

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 Schrodinger equation for $R(r) = \chi(r)/r$ is

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dr^2} - \frac{Ze^2}{r}\chi + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\chi = E\chi$$

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 the bouncing electron equation with the replacements

$$r \to y \quad , \quad Z \to \frac{1}{4}$$

Therefore, the solution for the bouncing electron ground sates is

$$\psi_1(y) = yR_{10}(y) = 2y\left(\frac{Z}{a}\right)^{3/2} e^{-Zy/a} \quad , \quad a = \frac{\hbar^2}{me^2}$$

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

$$\psi_{n,p_x,p_z}(x,y,z) = AR_{n0}(y)e^{i(p_x x + p_z z)/\hbar}$$

where A is the normalization factor.

7.7.34 Alkali Atoms

The alkali atoms have an electronic structure which resembles that of hydrogen. In particular, the spectral lines and chemical properties are largely determined by one electron(outside closed shells). A model for the potential in which this electron moves is

$$V(r) = -\frac{e^2}{r}\left(1 + \frac{b}{r}\right)$$

Solve the Schrodinger equation and calculate the energy levels.

The radial Schrodinger equation for the alkali atom is

$$\frac{\hbar^2}{2m}\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}\right)R_\ell(r) - \frac{e^2}{r}R_\ell(r) - \frac{e^2 b}{r^2}R_\ell(r) = ER_\ell(r)$$

This can be rewritten as

$$\frac{\hbar^2}{2m}\left(-\frac{d^2}{dr^2}+\frac{\bar{\ell}(\bar{\ell}+1)}{r^2}\right)R_\ell(r)-\frac{e^2}{r}R_\ell(r)=ER_\ell(r)$$

where

$$\bar{\ell}(\bar{\ell}+1)=\ell(\ell+1)-be^2\to\bar{\ell}=-\frac{1}{2}+\sqrt{\ell(\ell+1)-be^2+1/4}$$

The rewritten equation is just the hydrogen atom with $\ell\to\bar{\ell}$.

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* $n=k+\bar{\ell}+1$, which would not be an integer. The alkali energy levels then become

$$E=-\frac{e^2}{2a_0}\frac{1}{\left(n+\sqrt{(\ell+1/2)^2-be^2+1/4)}-\ell-1/2\right)^2}$$

Note that the energy levels depend on the angular momentum quantum number, ℓ, as well as the principal quantum number, n. We need to restrict the parameter $be^2\leq 1/4$, to ensure that all these energy levels are real.

The *accidental* degeneracy of the hydrogen atom has been lifted.

7.7.35 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

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left(\frac{2m}{\hbar^2}\left(E-V(r)\right)-\frac{\ell(\ell+1)}{r^2}\right)R=0$$

Substituting $R(r)=\chi(r)/r$ we have

$$\frac{d^2\chi}{dr^2}+\left[\frac{2m}{\hbar^2}\left(E-V(r)\right)-\frac{\ell(\ell+1)}{r^2}\right]\chi=0$$

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

$$\chi(r) = A\sin Kr + B\cos Kr$$
$$\chi(a) = 0 = A\sin Ka + B\cos Ka \rightarrow \tfrac{B}{A} = -\tan Ka$$

We choose

$$A = C\cos Ka \quad , \quad B = -C\sin Ka$$

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

$$R_{10}(r) = \sqrt{\frac{2}{b-a}}\frac{1}{r}\sin\frac{\pi(r-a)}{b-a} \text{ since ground state is } n=1$$

Finally, the fully normalized wave function is

$$\psi(\vec{r}) = R_{10}(r)Y_{00}(\Omega) = \frac{1}{\sqrt{4\pi}}\sqrt{\frac{2}{b-a}}\frac{1}{r}\sin\frac{\pi(r-a)}{b-a}$$

7.7.36 Logarithmic potential

A particle of mass m moves in the logarithmic potential

$$V(r) = C\ell n\left(\frac{r}{r_0}\right)$$

Show that:

(a) All the eigenstates have the same mean-squared velocity. Find this mean-squared velocity. Think Virial theorem!

We have

$$\langle \vec{v}^2 \rangle = \frac{1}{m^2}\langle \vec{p}^2 \rangle = \frac{1}{m^2}\int d^3r\psi^*(\vec{r})\vec{p}^2\psi(\vec{r})$$

For a stationary state, the virial theorem gives

$$\langle T \rangle = \frac{1}{2}\langle \vec{r}\cdot\nabla V(\vec{r})\rangle$$

Therefore,

$$\left\langle \vec{v}^2 \right\rangle = \frac{1}{m^2}\left\langle \vec{p}^2 \right\rangle = \frac{2}{m}\left\langle T \right\rangle = \frac{1}{m}\left\langle \vec{r}\cdot\nabla V(\vec{r}) \right\rangle notag \tag{7.2}$$
$$= \frac{1}{m}\int d^3r\, r\frac{d}{dr}\left(C\ell n\frac{r}{r_0}\right)\psi^*\psi = \frac{C}{m}\int d^3r\,\psi^*\psi = \frac{C}{m}$$

which is true for any eigenstate.

(b) The spacing between any two levels is independent of the mass m.

We have

$$\frac{\partial E_n}{\partial m} = \left\langle \frac{\partial \hat{H}}{\partial m} \right\rangle = \left\langle -\frac{\vec{p}^2}{2m^2} \right\rangle = -\frac{1}{2}\left\langle \vec{v}^2 \right\rangle = -\frac{C}{2m}$$

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.

7.7.37 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

$$V(x) = \begin{cases} -V_0 & 0 \le r \le r_0 \\ 0 & r > r_0 \end{cases}$$

(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

$$-\tfrac{\hbar^2}{2m}\tfrac{d^2\chi}{dr^2} - V_0\chi = E\chi \qquad 0 \le r \le r_0$$
$$-\tfrac{\hbar^2}{2m}\tfrac{d^2\chi}{dr^2} = E\chi \qquad r > r_0$$

with boundary condition $\chi(0) = 0$ and $\chi(\infty) =$ finite.

We can satisfy these conditions by choosing

$$\chi(r) = \sin\alpha r \qquad 0 \le r \le r_0$$
$$\chi(r) = Be^{-\beta r} \qquad r > r_0$$

where

$$\alpha = \frac{1}{\hbar}\sqrt{2m(E+V_0)} \quad , \quad \beta = \frac{1}{\hbar}\sqrt{-2mE}$$

Now at $r = r_)$, $\chi(r)$ and $d\chi)/dr$ are continuous, so that

$$\sin\alpha r_0 = Be^{-\beta r_0} \quad , \quad \alpha\cos\alpha r_0 = -B\beta e^{-\beta r_0}$$

which gives

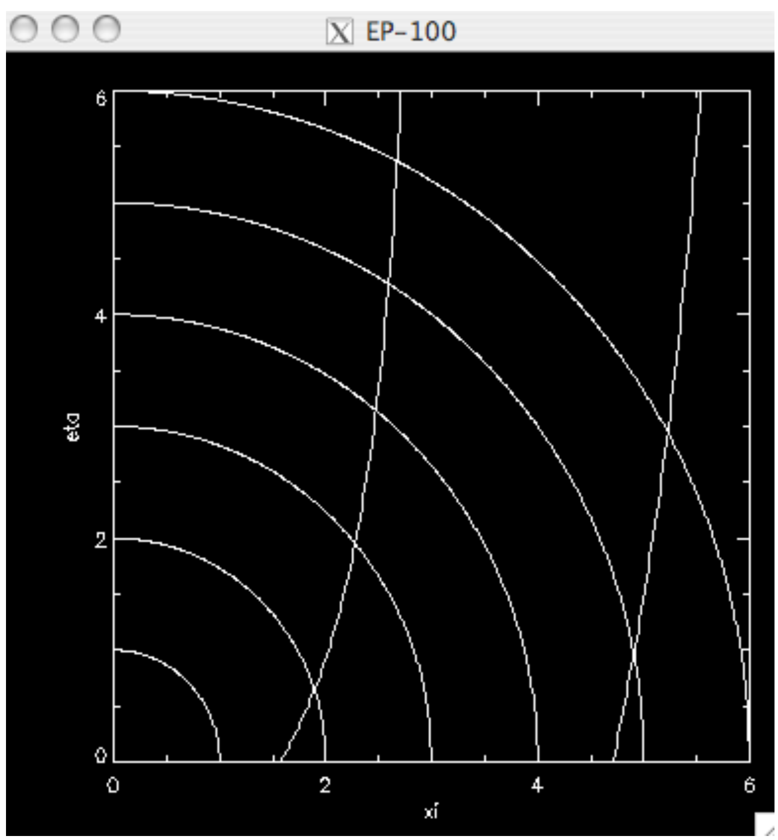
$$-\alpha\cot\alpha r_0 = \beta$$

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 ξ and η 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

$$\xi^2 + \eta^2 = \frac{2mV_0 r_0^2}{\hbar^2}$$

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

$$\frac{2mV_0 r_0^2}{\hbar^2} \geq \left(\frac{3\pi}{2}\right)^2 \rightarrow V_0 \geq \frac{9\pi^2\hbar^2}{8mr_0^2}$$

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

$$\begin{aligned}
&\xi^2 + \eta^2 = \left(\tfrac{3\pi}{2}\right)^2 \rightarrow \xi = \tfrac{3\pi}{2}\sqrt{1 - \left(\tfrac{2\beta r_o}{3\pi}\right)^2} \\
&-\xi \cot \xi = \eta \rightarrow -\tfrac{3\pi}{2}\sqrt{1 - \left(\tfrac{2\eta}{3\pi}\right)^2} \cot\left(\tfrac{3\pi}{2}\sqrt{1 - \left(\tfrac{2\eta}{3\pi}\right)^2}\right) = \eta \\
&-\tfrac{2\eta}{3\pi} \tan\left(\tfrac{3\pi}{2}\sqrt{1 - \left(\tfrac{2\eta}{3\pi}\right)^2}\right) = \sqrt{1 - \left(\tfrac{2\eta}{3\pi}\right)^2}
\end{aligned}$$

or

$$\begin{aligned}
f(\eta) &= \sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2} + \frac{2\eta}{3\pi} \tan\left(\frac{3\pi}{2}\sqrt{1 - \left(\frac{2\eta}{3\pi}\right)^2}\right) \\
&= \sqrt{1 - 0.045\eta^2} + 0.212\eta \tan\left(4.712\sqrt{1 - 0.045\eta^2}\right) = 0
\end{aligned}$$

If we solve the last equation numerically (find the zeroes of $f(\eta)$) to find η, we get $\eta = 0,\ 4.444$, and then the energy is given by

$$\beta = \frac{\eta}{r_0} \quad , \quad E = -\frac{\hbar^2}{2m}\beta^2 = -\frac{\hbar^2}{2m}\frac{\eta^2}{r_0^2}$$

7.7.38 In magnetic and electric fields

A point particle of mass m and charge q moves in spatially constant crossed magnetic and electric fields $\vec{B} = B_0\hat{z}$ and $\vec{\mathcal{E}} = \mathcal{E}_0\hat{x}$.

(a) Solve for the complete energy spectrum.

We choose a gauge such that $\vec{A} = B_0 x\hat{e}_y$ and $\phi = -\varepsilon_0 x$ so that $\nabla \times \vec{A} = B_0\hat{e}_z$ and $-\nabla\phi = \varepsilon_0\hat{e}_x$. We then have

$$\hat{H} = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}(\vec{r})\right)^2 + q\phi = \frac{1}{2m}\left(\hat{p}_x^2 + \left(\hat{p}_y - \frac{qB_0}{c}\hat{x}\right)^2 + \hat{p}_z^2\right) - q\varepsilon_0\hat{x}$$

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

$$\begin{aligned}\hat{H} &= \frac{1}{2m}\left(\hat{p}_x^2 + \left(p_y - \frac{qB_0}{c}\hat{x}\right)^2 + p_z^2\right) - q\varepsilon_0\hat{x} \\ &= \frac{1}{2m}\hat{p}_x^2 + \frac{q^2B_0^2}{2mc^2}\left(\hat{x} - \frac{cp_y}{qB_0} - \frac{mc^2\varepsilon_0}{qB_0^2}\right)^2 + \frac{1}{2m}\hat{p}_z^2 - \frac{mc^2\varepsilon_0^2}{2B_0^2} - \frac{cp_y\varepsilon_0}{B_0}\end{aligned}$$

Now let

$$\hat{p}_\xi = \hat{p}_x \quad , \quad \hat{\xi} = \hat{x} - \frac{cp_y}{qB_0} - \frac{mc^2\varepsilon_0}{qB_0^2} \quad , \quad \omega = \frac{|e|\, B_0}{mc}$$

We then have

$$\hat{H} = \frac{1}{2m}\hat{p}_\xi^2 + \frac{1}{2}m\omega^2\hat{\xi}^2 + \frac{1}{2m}\hat{p}_z^2 - \frac{mc^2\varepsilon_0^2}{2B_0^2} - \frac{cp_y\varepsilon_0}{B_0}$$

Now,

$$[\hat{x}, \hat{p}_x] = i\hbar \to \left[\hat{\xi}, \hat{p}_\xi\right] = i\hbar \text{ (a new pair of conjugate variables)}$$

This represents a simple harmonic oscillator. Therefore,

$$E_n = (n + 1/2)\hbar\omega + \frac{1}{2m}\hat{p}_z^2 - \frac{mc^2\varepsilon_0^2}{2B_0^2} - \frac{cp_y\varepsilon_0}{B_0} \quad , \quad n = 0, 1, 2, ...$$

(b) Find the expectation value of the velocity operator

$$\vec{v} = \frac{1}{m}\vec{p}_{mechanical}$$

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

$$\vec{v} = \frac{1}{m}\vec{P}_{mechanical} = \frac{1}{m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)$$

Therefore,

$$\langle \vec{v} \rangle = \frac{1}{m}\langle \vec{p} \rangle - \frac{q}{c}\left\langle \vec{A} \right\rangle = -\frac{q}{c}\left\langle \vec{A} \right\rangle = -\frac{qB_0}{mc}\langle \hat{x} \rangle \hat{e}_y$$

But,

$$\langle \hat{x} \rangle = \left\langle \hat{\xi} \right\rangle + \frac{cp_y}{qB_0} + \frac{mc^2\varepsilon_0}{qB_0^2} = \frac{mc^2\varepsilon_0}{qB_0^2}$$

since

$$\left\langle \hat{\xi} \right\rangle = 0 \text{ for simple harmonic motion}$$

Finally,

$$\langle \vec{v} \rangle = -\frac{qB_0}{mc}\langle \hat{x} \rangle \hat{e}_y = -\frac{c\varepsilon_0}{B_0}\hat{e}_y$$

7.7.39 Extra(Hidden) Dimensions

Lorentz Invariance with Extra Dimensions

If string theory is correct, we must entertain the possibility that space-time has more than four dimensions. The number of time dimensions must be kept equal to one - it seems very difficult, if not altogether impossible, to construct a consistent theory with more than one time dimension. The extra dimensions must therefore be spatial.

Can we have Lorentz invariance in worlds with more than three spatial dimensions? The answer is yes. Lorentz invariance is a concept that admits a very natural generalization to space-times with additional dimensions.

We first extend the definition of the invariant interval ds^2 to incorporate the additional space dimensions. In a world of five spatial dimensions, for example, we would write

$$ds^2 = c^2dt^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2 - (dx^4)^2 - (dx^5)^2 \tag{7.3}$$

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 7.4 below.

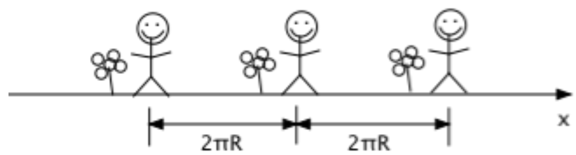


Figure 7.4: Multiple friends

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 $2\pi R$:

$$P_1 \sim P_2 \leftrightarrow x(P_1) = x(P_2) + 2\pi R n \quad , \quad n \in \mathrm{Z} \tag{7.4}$$

This is precise, but somewhat cumbersome, notation. With no risk of confusion, we can simply write

$$x \sim x + 2\pi R \tag{7.5}$$

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 (7.3) as shown in Figure 7.5 below.

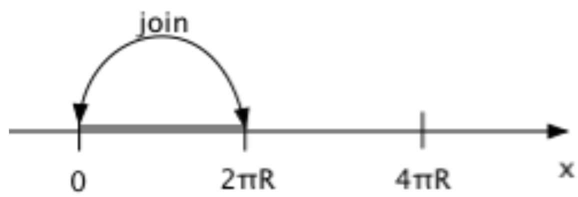


Figure 7.5: Fundamental domain

A fundamental domain is a subset of the entire space that satisfies two conditions:

(1) no two points in are identified

(2) any point in the entire space is related by the identification to some point in the fundamental domain

Whenever possible, as we did here, the fundamental domain is chosen to be a connected region. To build the space implied by the identification, we take the fundamental domain together with its boundary, and implement the identifications on the boundary. In our case, the fundamental domain together with its boundary is the segment $0 \leq x \leq 2\pi R$. In this segment we identify the point $x = 0$ with the point $x = 2\pi R$. The result is the circle.

A circle of radius R can be represented in a two-dimensional plane as the set of points that are a distance R from a point called the center of the circle. Note that the circle obtained above has been constructed directly, without the help of any two-dimensional space. For our circle, there is no point, anywhere, that represents the center of the circle. We can still speak, figuratively, of the radius R of the circle, but in our case, the radius is simply the quantity which multiplied by 2π gives the total length of the circle.

On the circle, the coordinate x is no longer a good coordinate. The coordinate x is now either multi-valued or discontinuous. This is a problem with any coordinate on a circle. Consider using angles to assign coordinates on the unit circle as shown in Figure 7.6 below.

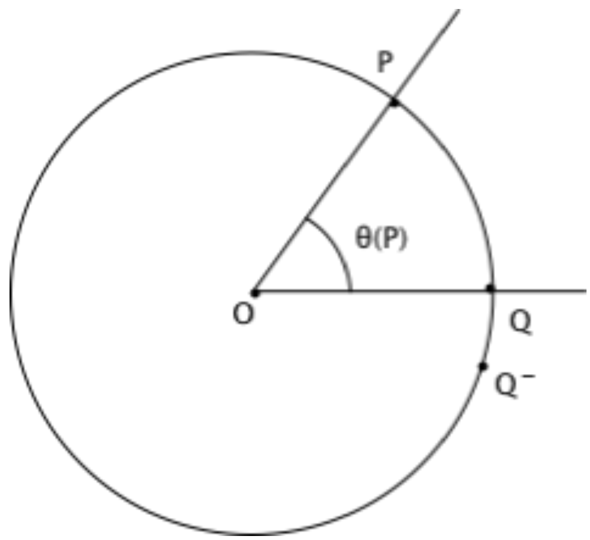


Figure 7.6: Unit circle identification

Fix a reference point Q on the circle, and let O denote the center of the circle. To any point P on the circle we assign as a coordinate the angle $\theta(P) = angle(POQ)$. This angle is naturally multi-valued. The reference point Q, for example, has $\theta(Q) = 0°$ and $\theta(Q) = 360°$. If we force angles to be single-valued by restricting $0° \leq \theta \leq 360°$, for example, then they become discontinuous. Indeed, two nearby points, Q and Q^-, then have very different angles $\theta(Q) = 0°$, while $\theta(Q^-) \sim 360°$. It is easier to work with multi-valued coordinates than it is to work with discontinuous ones.

If we have a world with several open dimensions, then we can apply the identification (7.3) to one of the dimensions, while doing nothing to the others. The dimension described by x turns into a circle, and the other dimensions remain open. It is possible, of course, to make more than one dimension compact.

Consider the example, the (x, y) plane, subject to two identifications,

$$x \sim x + 2\pi R \quad , \quad y \sim y + 2\pi R$$

It is perhaps clearer to show both coordinates simultaneously while writing the identifications. In that fashion, the two identifications are written as

$$(x, y) \sim (x + 2\pi R, y) \quad , \quad (x, y) \sim (x, y + 2\pi R) \tag{7.6}$$

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 7.7 below.

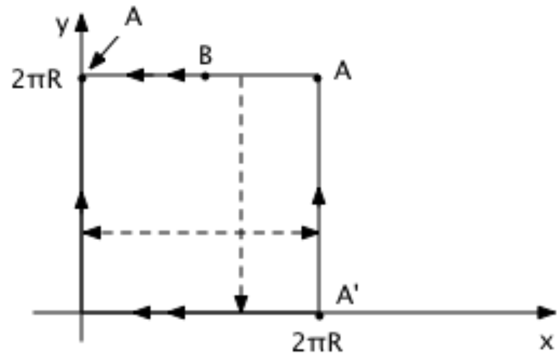


Figure 7.7: Fundamental domain = square

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 (7.4). This results in the cylinder shown in Figure 7.8 below.

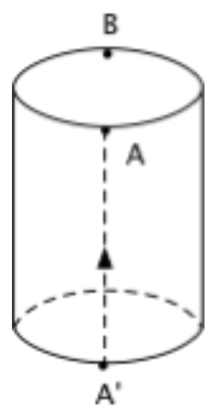


Figure 7.8: Square → cylinder

The horizontal edges are identified because they correspond to points of the form $(x, 0)$ and $(x, 2\pi R)$, which are identified by the second equation in (7.4). The resulting space is a two-dimensional torus.

We can visualize this process in Figure 7.9 below.

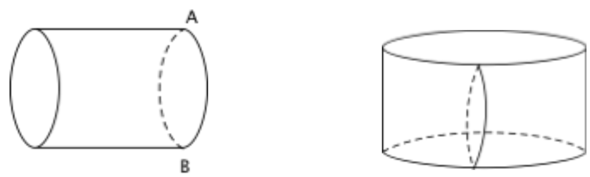


Figure 7.9: 2-dimensional torus

or in words, the torus is visualized by taking the fundamental domain (with its boundary) and gluing the vertical edges as their identification demands. The result is first (vertical) cylinder shown above (the gluing seam is the dashed line). In this cylinder, however, the bottom circle and the top circle must also be glued, since they are nothing other than the horizontal edges of the fundamental domain. To do this with paper, you must flatten the cylinder and then roll it up and glue the circles. The result looks like a flattened doughnut. With a flexible piece of garden hose, you could simply identify the two ends and obtain the familiar picture of a torus.

We have seen how to compactify coordinates using identifications. Some compact spaces are constructed in other ways. In string theory, however, compact spaces that arise from identifications are particularly easy to work with.

Sometimes identifications have fixed points, points that are related to themselves by the identification. For example, consider the real line parameterized by the coordinate x and subject to the identification $x \sim -x$. The point $x = 0$ is the unique fixed point of the identification. A fundamental domain can be chosen to be the half-line $x \geq 0$. Note that the boundary point $x = 0$ must be included in the fundamental domain. The space obtained by the above identification is in fact the fundamental domain $x \geq 0$. This is the simplest example of an *orbifold*, a space obtained by identifications that have fixed points. This orbifold is called an R^1/Z_2 orbifold. Here R^1 stands for the (one-dimensional) real line, and Z_2 describes a basic property of the identification when it is viewed as the transformation $x \to -x$ - if applied twice, it gives back the original coordinate.

Quantum Mechanics and the Square Well

The fundamental relation governing quantum mechanics is

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

In three spatial dimensions the indices i and j run from 1 to 3. The generalization of quantum mechanics to higher dimensions is straightforward. With d spatial dimensions, the indices simply run over the d possible values.

To set the stage for for the analysis of small extra dimensions, let us review the standard quantum mechanics problem involving and infinite potential well.

The time-independent Schrodinger equation(in one-dimension) is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

In the infinite well system we have

$$V(x) = \begin{cases} 0 & \text{if } x \in (0,a) \\ \infty & \text{if } x \notin (0,a) \end{cases}$$

When $x \in (0,a)$, the Schrodinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

The boundary conditions $\psi(0) = \psi(a) = 0$ give the solutions

$$\psi_k(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{k\pi x}{a}\right) \quad , \quad k = 1, 2, ..., \infty$$

The value $k = 0$ is not allowed since it would make the wave-function vanish everywhere. The corresponding energy values are

$$E_k = \frac{\hbar^2}{2m}\left(\frac{k\pi}{a}\right)^2$$

Square Well with Extra Dimensions

We now add an extra dimension to the square well problem. In addition to x, we include a dimension y that is curled up into a small circle of radius R. In other words, we make the identification

$$(x, y) \sim (x, y + 2\pi R)$$

The original dimension x has not been changed(see Figure 7.10 below). In the figure, on the left we have the original square well potential in one dimension. Here the particle lives on the the line segment shown and on the right, in the (x, y) plane the particle must remain in $0 < x < a$. The direction y is identified as $y \sim y + 2\pi R$.

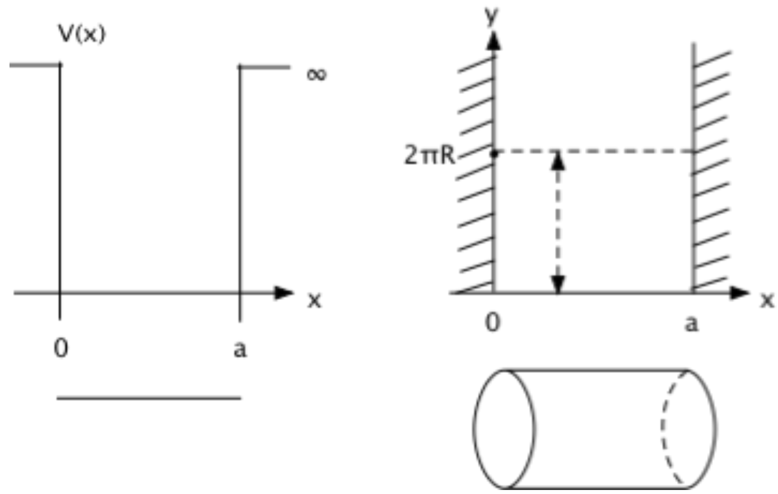


Figure 7.10: Square well with compact hidden dimension

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

$$\alpha_k(x)=c_k\sin\left(\tfrac{k\pi x}{a}\right)$$
$$\beta_l(y)=a_l\sin\left(\tfrac{ly}{R}\right)+b_l\cos\left(\tfrac{ly}{R}\right)$$

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 $k=1,2,3,....$ 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 ψ_{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 eiegnstate of the original problem where

$$\frac{k\pi}{a} \sim \frac{1}{R} \to k \sim \frac{1}{\pi}\frac{a}{R}$$

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.

he quantum mechanics of a string introduces new features not present here. For an extra dimension much smaller than the already small string length ℓ_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 ℓ_s.

7.7.40 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

$$H = A + B\vec{L}\cdot\vec{S} + C\vec{L}\cdot\vec{L}$$

What are the values of energy for each of the different states of total angular momentum in terms of the constants A, B, and C?

We have $\vec{J} = \vec{L} + \vec{S}$, $L = 2$, $S = 1/2$. Thus, the possible values for j are 5/2 and 3/2 ($\ell + s \geq j \geq |\ell - s|$).

Now
$$H|j,m\rangle = (A + B\vec{L}\cdot\vec{S} + C\vec{L}\cdot\vec{L})|j,m\rangle$$
where $|j,m\rangle = |\ell, s; j, m\rangle =$.

Then, we have
$$\vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$$

$$\begin{aligned}\vec{L}\cdot\vec{S}\,|\ell,s;j,m\rangle &= \frac{1}{2}(J^2 - L^2 - S^2)\,|\ell,s;j,m\rangle \\ &= \frac{1}{2}\hbar^2(j(j+1) - \ell(\ell+1) - s(s+1))\,|\ell,s;j,m\rangle = \frac{1}{2}\hbar^2\left(j(j+1) - g - \frac{3}{4}\right)|\ell,s;j,m\rangle\end{aligned}$$

$$\vec{L}\cdot\vec{L} = L^2$$
$$\vec{L}\cdot\vec{L} = L^2\,|\ell,s;j,m\rangle = \hbar^2\ell(\ell+1)\,|\ell,s;j,m\rangle = 6\hbar^2\,|\ell,s;j,m\rangle$$

so that
$$H|j,m\rangle = (A + \frac{1}{2}B\hbar^2\left(j(j+1) - g - \frac{3}{4}\right) + 6C\hbar^2)\,|j,m\rangle = E_{jm}\,|j,m\rangle$$

Thus,
$$\text{For } j = \frac{5}{2} \quad E_{jm} = A + B\hbar^2 + 6C\hbar^2 \quad \text{independent of } m$$
$$\text{For } j = \frac{3}{2} \quad E_{jm} = A - \frac{3}{2}B\hbar^2 + 6C\hbar^2 \quad \text{independent of } m$$

7.7.41 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:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Calculate the eigenvalues of $\vec{S}$. The vector $\vec{sigma}$ is defined as a vector whose components aren 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 ± 1. To prove thsi, 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 ψ as a 2-component vector

$$\psi = \begin{pmatrix} A \\ B \end{pmatrix}$$

we get the two equations

$$\begin{aligned} A\cos\theta + B\sin\theta &= \pm A \\ A\sin\theta - B\cos\theta &= \pm B \end{aligned}$$

These give

$$\begin{aligned} \tfrac{A}{B} &= \sin\theta(\pm 1 - \cos\theta) \\ \tfrac{A}{B} &= \tfrac{\cos\theta \pm 1}{\sin\theta} \end{aligned}$$

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,

$$\psi_\pm = N_\pm \begin{pmatrix} \sin\theta \\ \pm 1 - \cos\theta \end{pmatrix}$$

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 α and β come from the scalar product of $|\uparrow\rangle$ with ψ_+ and ψ_-, i.e.,

$$\alpha = \langle\uparrow|+\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} N_+ \begin{pmatrix} \sin\theta \\ \pm 1 - \cos\theta \end{pmatrix} = N_+ \sin\theta$$

and

$$\beta = \langle\uparrow|-\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} N_- \begin{pmatrix} \sin\theta \\ \pm - 1 - \cos\theta \end{pmatrix} = N_- \sin\theta$$

The ratio of the two beam intensities is given by

$$\frac{|\alpha|^2}{|\beta|^2} = \frac{|N_+|^2}{|N_-|^2} = \frac{1+\cos\theta}{1-\cos\theta} = \cot^2\left(\frac{\theta}{2}\right)$$

7.7.42 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.

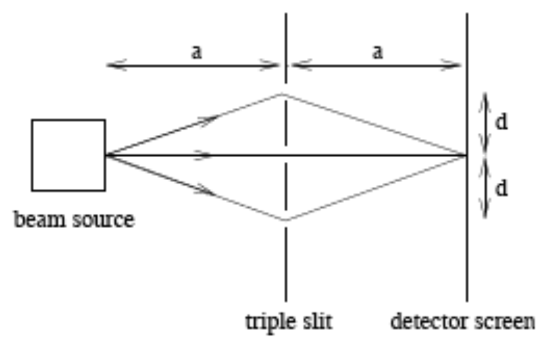


Figure 7.11: Triple-Slit Setup

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.

7.7.43 Cylindrical potential

The Hamiltonian is given by

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2\mu} + V(\hat{\rho})$$

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

(a) Use symmetry arguments to establish that both $\hat{p}_z$ and $\hat{L}_z$, the $z-$component of the linear and angular momentum operators, respectively, commute with $\hat{H}$.

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 φ), 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

$$\langle \vec{r} \mid E, p_z, m\rangle = \frac{e^{ip_z z/\hbar}}{\sqrt{2\pi\hbar}} \frac{e^{im\varphi}}{\sqrt{2\pi}} R(\rho)$$

(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 μ 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

$$E_{n\alpha} = \frac{\hbar^2}{2\mu a^2} z_{n\alpha}^2 \quad , \quad z_{n\alpha} = n^{th} \; zero \; of \; J_\alpha$$

$$\langle \vec{r}|\, \hat{H} \,|E, p_z, m\rangle = \left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(\hat{\rho})\right) \langle \vec{r} \mid E, p_z, m\rangle = E \,\langle \vec{r} \mid E, p_z, m\rangle$$

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

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial R}{\partial \rho}\right) + \frac{\hbar^2}{2\mu}\frac{m^2}{\rho^2} R + \frac{p_z^2}{2\mu} R + V(\rho) R\right) \frac{e^{ip_z z/\hbar}}{\sqrt{2\pi\hbar}} \frac{e^{im\varphi}}{\sqrt{2\pi}} = E \frac{e^{ip_z z/\hbar}}{\sqrt{2\pi\hbar}} \frac{e^{im\varphi}}{\sqrt{2\pi}} R$$
$$-\frac{\hbar^2}{2\mu}\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial R}{\partial \rho}\right) + \frac{\hbar^2}{2\mu}\frac{m^2}{\rho^2} R + \frac{p_z^2}{2\mu} R + V(\rho) R = E R$$

Now rearranging and using

$$\lambda^2 = \frac{2\mu E}{\hbar^2} \quad , \quad p_z = \hbar k$$

we have

$$\rho^2 \frac{d^2 R}{d\rho^2} + \rho \frac{dR}{d\rho} + \left(\lambda^2 \rho^2 - (m^2 + k^2)\right) R - \frac{2\mu}{\hbar^2}\rho^2 V(\rho) R = 0$$

(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 $\rho < a$

$$\rho^2 \frac{d^2R}{d\rho^2} + \rho \frac{dR}{d\rho} + \left(\lambda^2\rho^2 - (m^2 + k^2)\right) R = 0 \quad and \quad R(a) = 0$$

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 2^{nd} kind since they are not finite at $\rho = 0$.

The boundary condition becomes $J_\alpha(\lambda a) = 0$ so that $\lambda a =$ a zero of the Bessel function of order α.

Therefore,

$$E_{n\alpha} = \frac{\hbar^2}{2\mu a^2} z_{n\alpha}^2 \quad , \quad z_{n\alpha} = n^{th}\ zero\ of\ J_\alpha$$

When $p_z = \hbar k = 0 = m \to \alpha = 0$ we are looking for the zeroes of J_0. The three lowest energy eigenvalues are then

$$\begin{aligned} E_1 &= \tfrac{\hbar^2}{2\mu a^2}(2.4048)^2 \\ E_2 &= \tfrac{\hbar^2}{2\mu a^2}(5.5201)^2 \\ E_3 &= \tfrac{\hbar^2}{2\mu a^2}(8.6537)^2 \end{aligned}$$

(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

$$\begin{aligned} J_0(z) = 0 &\to z = 2.40\,,\ 5.52\,,\ 8.65 \\ J_1(z) = 0 &\to z = 3.83\,,\ 7.02\,,\ 10.17 \\ J_2(z) = 0 &\to z = 5.14\,,\ 8.42\,,\ 11.62 \end{aligned}$$

and therefore the three lowest energies are

$$\begin{aligned} E_1 &= \tfrac{\hbar^2}{2\mu a^2}(2.4048)^2 \quad p_z = 0, m = 0 \to 1^{st}\ zero\ of\ J_0 \\ E_2 &= \tfrac{\hbar^2}{2\mu a^2}(3.8317)^2 \quad p_z = 0, m = 1 \to 1^{st}\ zero\ of\ J_1 \\ E_3 &= \tfrac{\hbar^2}{2\mu a^2}(5.1356)^2 \quad p_z = 0, m = 2 \to 1^{st}\ zero\ of\ J_2 \end{aligned}$$

7.7.44 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 $A > 0$, $B > 0$, $|\lambda| < 1$. μ is arbitrary. Find the energy eigenvalues.

We choose two new variables

$$u = \frac{1}{\sqrt{2}}(x+y) \quad , \quad t = \frac{1}{\sqrt{2}}(x-y)$$
$$x = \frac{u+t}{\sqrt{2}} \quad , \quad y = \frac{u-t}{\sqrt{2}}$$

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

$$\frac{\partial}{\partial x} = \frac{1}{\sqrt{2}}\frac{\partial}{\partial u} + \frac{1}{\sqrt{2}}\frac{\partial}{\partial t}$$
$$\to \frac{\partial^2}{\partial x^2} = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\frac{\partial^2}{\partial u^2} + \frac{1}{\sqrt{2}}\frac{\partial^2}{\partial u \partial t}\right) + \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\frac{\partial^2}{\partial t^2} + \frac{1}{\sqrt{2}}\frac{\partial^2}{\partial u \partial t}\right)$$

$$\frac{\partial}{\partial y} = \frac{1}{\sqrt{2}}\frac{\partial}{\partial u} - \frac{1}{\sqrt{2}}\frac{\partial}{\partial t}$$
$$\to \frac{\partial^2}{\partial y^2} = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\frac{\partial^2}{\partial u^2} - \frac{1}{\sqrt{2}}\frac{\partial^2}{\partial u \partial t}\right) - \frac{1}{\sqrt{2}}\left(-\frac{1}{\sqrt{2}}\frac{\partial^2}{\partial t^2} + \frac{1}{\sqrt{2}}\frac{\partial^2}{\partial u \partial t}\right)$$

so that

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial z^2}$$

and the Schrodinger equation becomes

$$\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial z^2}\right)\varphi(u,t,z) + \frac{2m}{\hbar^2}\left(E - V(u,t,z)\right)\varphi(u,t,z) = 0$$

We now separate variables. Substituting $\varphi(u,t,z) = U(u)T(t)Z(z)$ gives

$$\frac{\partial^2 U}{\partial u^2} + \frac{2m}{\hbar^2}\left(E_1 + A(1+\lambda)u^2\right)U = 0$$
$$\frac{\partial^2 T}{\partial t^2} + \frac{2m}{\hbar^2}\left(E_2 - A(1-\lambda)t^2\right)T = 0$$
$$\frac{\partial^2 Z}{\partial z^2} + \frac{2m}{\hbar^2}\left(E_3 - B(z^2+2\mu z)\right)Z = 0$$

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,

$$E_1 = (n_1 + 1/2)\hbar\omega_1 \quad , \quad \omega_1 = \sqrt{\frac{2A}{m}(1+\lambda)}$$
$$E_2 = (n_2 + 1/2)\hbar\omega_2 \quad , \quad \omega_2 = \sqrt{\frac{2A}{m}(1-\lambda)}$$
$$E_3 = (n_3 + 1/2)\hbar\omega_3 - B\mu^2 \quad , \quad \omega_3 = \sqrt{\frac{2B}{m}}$$

where n_1 , n_2 , $n_3 = 0, 1, 2, 3, ...$

(b) Now consider the following modified problem with a new potential

$$V_{new} = \begin{cases} V(x,y,z) & z > -\mu \text{ and any x and y} \\ +\infty & z < -\mu \text{ and any x and y} \end{cases}$$

Find the ground state energy.

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

$$Z(z) = H_{n_3}(\zeta)e^{-\zeta^2} \quad , \quad \zeta = \left(\frac{2mB}{\hbar^2}\right)^{1/4}(z+\mu)$$

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 $n_3 = 1, 3, 5, ...$

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

$$E_0 = \frac{1}{2}\hbar(\omega_1 + \omega_2 + \omega_3) - B\mu^2$$

The new ground state energy is

$$E_0' = \frac{1}{2}\hbar(\omega_1 + \omega_2 + 3\omega_3) - B\mu^2$$

7.7.45 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 θ relative to the $z-$axis. Both devices only transmit the uppermost beam. What fraction of the particles entering the second device will leave the second device?

As preparation we determine the eigenvectors corresponding to the eigenvalues $m_y\hbar$, $m_y = 1, 0, -1$ of S_y. From $S_y\left|m_y\right\rangle = m_y\hbar\left|m_y\right\rangle$ 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

$$\begin{aligned}&-i\tfrac{\hbar}{\sqrt{2}}b = m_y\hbar a\\ &i\tfrac{\hbar}{\sqrt{2}}a - i\tfrac{\hbar}{\sqrt{2}}c = m_y\hbar b\\ &i\tfrac{\hbar}{\sqrt{2}}b = m_y\hbar c\end{aligned}$$

These give

$$|m_y = \pm 1\rangle = \frac{1}{2}\begin{pmatrix}1\\ \pm\sqrt{2}i\\ -1\end{pmatrix} \quad , \quad |m_y = 0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}$$

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 θ 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 SGz 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:

$$\begin{aligned}|\psi\rangle &= \sum_{m_y} e^{iS_y\theta/\hbar}\,|m_y\rangle\,\langle m_y\,|\,m_z = 1\rangle\\ &= e^{i\theta}\,|m_y = 1\rangle\,\langle m_y = 1\,|\,m_z = 1\rangle + |m_y = 0\rangle\,\langle m_y = 0\,|\,m_z = 1\rangle\\ &\quad + e^{-i\theta}\,|m_y = -1\rangle\,\langle m_y = -1\,|\,m_z = 1\rangle\end{aligned}$$

The amplitude of the spin-up state exiting the second device is

$$\begin{aligned}\langle m_z = 1\,|\,\psi\rangle &= e^{i\theta}|\,\langle m_y = 1\,|\,m_z = 1\rangle\,|^2 + |\,\langle m_y = 0\,|\,m_z = 1\rangle\,|^2\\ &\quad e^{-i\theta}|\,\langle m_y = -1\,|\,m_z = 1\rangle\,|^2\\ &= \frac{e^{i\theta}}{4} + \frac{1}{2} + \frac{-e^{i\theta}}{4} = \frac{1+\cos\theta}{2}\end{aligned}$$

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

$$N_{-1}(\theta) = \frac{(1-\cos\theta)^2}{4} = N_{+1}(\pi - \theta) \quad , \quad N_0(\theta) = \frac{\sin^2\theta}{2}$$

so that $N_{+1} + N_{-1} + N_0 = 1$.

7.7.46 Three Spherical Harmonics

As we see, often we need to calculate an integral of the form

$$\int d\Omega Y^*_{\ell_3 m_3}(\theta,\varphi) Y_{\ell_2 m_2}(\theta,\varphi) Y_{\ell_1 m_1}(\theta,\varphi)$$

This can be interpreted as the matrix element $\langle \ell_3 m_3 | \hat{Y}^{(\ell_2)}_{m_2} | \ell_1 m_1 \rangle$, where $\hat{Y}^{(\ell_2)}_{m_2}$ is an irreducible tensor operator.

(a) Use the Wigner-Eckart theorem to determine the restrictions on the quantum numbers so that the integral does not vanish.

We have

$$\begin{aligned} \langle \ell_3 m_3 | \hat{Y}^{(\ell_2)}_{m_2} | \ell_1 m_1 \rangle &= \int d\Omega Y^*_{\ell_3 m_3}(\theta,\varphi) Y_{\ell_2 m_2}(\theta,\varphi) Y_{\ell_1 m_1}(\theta,\varphi) \\ &= \langle \ell_3 \| \hat{Y}^{(\ell_2)} \| \ell_1 \rangle \langle \ell_3 m_3 \mid \ell_2 m_2 \ell_1 m_1 \rangle \end{aligned}$$

where we have used the Wigner-Eckart theorem.

Thus, this integral vanishes unless

$$\begin{aligned} &m_3 = m_2 + m_1 \\ &|\ell_2 - \ell_1| \leq \ell_3 \leq \ell_2 + \ell_1 \end{aligned}$$

(b) Given the *addition rule* for Legendre polynomials:

$$P_{\ell_1}(\mu) P_{\ell_2}(\mu) = \sum_{\ell_3} \langle \ell_3 0 \mid \ell_1 0 \ell_2 0 \rangle^2 P_{\ell_3}(\mu)$$

where $\langle \ell_3 0 \mid \ell_1 0 \ell_2 0 \rangle$ is a Clebsch-Gordon coefficient. Use the Wigner-Eckart theorem to prove

$$\begin{aligned} &\int d\Omega Y^*_{\ell_3 m_3}(\theta,\varphi) Y_{\ell_2 m_2}(\theta,\varphi) Y_{\ell_1 m_1}(\theta,\varphi) \\ &\quad = \sqrt{\frac{(2\ell_2+1)(2\ell_1+1)}{4\pi(2\ell_3+1)}} \langle \ell_3 0 \mid \ell_1 0 \ell_2 0 \rangle \langle \ell_3 m_3 \mid \ell_2 m_2 \ell_1 m_1 \rangle \end{aligned}$$

HINT: Consider $\langle \ell_3 0 | \hat{Y}^{(\ell_2)}_0 | \ell_1 0 \rangle$.

Consider

$$\langle \ell_3 0 | \hat{Y}^{(\ell_2)}_0 | \ell_1 0 \rangle = \int d\Omega Y^*_{\ell_3 0}(\theta,\varphi) Y_{\ell_2 0}(\theta,\varphi) Y_{\ell_1 0}(\theta,\varphi)$$

Now

$$Y^{(\ell)}_0 = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos\theta)$$

where $P_\ell(\cos\theta)$ is the Legendre polynomial. This implies that

$$\langle \ell_3 0 | \hat{Y}_0^{(\ell_2)} | \ell_1 0 \rangle = \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{(4\pi)^3}} \int d\Omega P_{\ell_3}(\cos\theta) P_{\ell_2}(\cos\theta) P_{\ell_1}(\cos\theta)$$

Now

$$P_{\ell_1}(\cos\theta) P_{\ell_2}(\cos\theta) = \sum_{\ell'} \langle \ell' 0 \mid \ell_1 0 \ell_2 0 \rangle^2 P_{\ell'}(\cos\theta)$$

Therefore,

$$\begin{aligned}
\int d\Omega Y_{\ell_3 0}^*(\theta,\varphi) Y_{\ell_2 0}(\theta,\varphi) Y_{\ell_1 0}(\theta,\varphi) &= \sum_{\ell'} \langle \ell' 0 \mid \ell_2 0 \ell_2 0 \rangle^2 \int d\Omega P_{\ell_3}(\cos\theta) P_{\ell'}(\cos\theta) \\
&= \sum_{\ell'} \langle \ell' 0 \mid \ell_2 0 \ell_2 0 \rangle^2 \int 2\pi d(\cos\theta) P_{\ell_3}(\cos\theta) P_{\ell'}(\cos\theta) \\
&= \sum_{\ell'} \langle \ell' 0 \mid \ell_2 0 \ell_2 0 \rangle^2 \frac{4\pi}{2\ell_3+1} \delta_{\ell_3 \ell'}
\end{aligned}$$

Therefore,

$$\begin{aligned}
\langle \ell_3 0 | \hat{Y}_0^{(\ell_2)} | \ell_1 0 \rangle &= \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell_3+1)}} \langle \ell_3 0 \mid \ell_1 0 \ell_2 0 \rangle^2 \\
&= \langle \ell_3 \| \hat{Y}^{(\ell_2)} \| \ell_1 \rangle \langle \ell_3 0 \mid \ell_1 0 \ell_2 0 \rangle
\end{aligned}$$

This implies that we can solve for the reduced matrix element. Putting it all together, we have

$$\begin{aligned}
&\int d\Omega Y_{\ell_3 m_3}^*(\theta,\varphi) Y_{\ell_2 m_2}(\theta,\varphi) Y_{\ell_1 m_1}(\theta,\varphi) \\
&= \sqrt{\frac{(2\ell_2+1)(2\ell_1+1)}{4\pi(2\ell_3+1)}} \langle \ell_3 0 \mid \ell_1 0 \ell_2 0 \rangle \langle \ell_3 m_3 \mid \ell_2 m_2 \ell_1 m_1 \rangle
\end{aligned}$$

7.7.47 Spin operators ala Dirac

Show that

$$\begin{aligned}
\hat{S}_z &= \frac{\hbar}{2} |z+\rangle \langle z+| - \frac{\hbar}{2} |z-\rangle \langle z-| \\
\hat{S}_+ &= \hbar |z+\rangle \langle z-| \quad , \quad \hat{S}_- = \hbar |z-\rangle \langle z+|
\end{aligned}$$

We have the general spectral decomposition of an operator

$$\hat{Q} = \sum_k Q_k |Q_k\rangle \langle Q_k| \quad , \quad \hat{Q} |Q_k\rangle = Q_k |Q_k\rangle$$

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

$$\begin{aligned}
\hat{S}_x &= \frac{\hbar}{2}|+x\rangle\langle +x| - \frac{\hbar}{2}|-x\rangle\langle -x| \\
&= \frac{\hbar}{2}\left(\frac{1}{2}(|+z\rangle + |-z\rangle)(\langle +z| + \langle -z|) - \frac{1}{2}(|+z\rangle - |-z\rangle)(\langle +z| - \langle -z|)\right) \\
&= \frac{\hbar}{2}|+z\rangle\langle -z| + \frac{\hbar}{2}|-z\rangle\langle +z|
\end{aligned}$$

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

$$\hat{S}_\pm = \frac{\hat{S}_x \pm i\hat{S}_y}{2} = \hbar|\pm z\rangle\langle \mp z|$$

Some other checks:we find

$$\begin{aligned}
&\hat{S}_z|\pm z\rangle = \pm\tfrac{\hbar}{2}|\pm z\rangle \\
&\hat{S}_+|+z\rangle = 0 \\
&\hat{S}_-|+z\rangle = \hbar|-z\rangle \\
&\hat{S}_+|-z\rangle = \hbar|+z\rangle \\
&\hat{S}_-|-z\rangle = 0
\end{aligned}$$

which are all consistent with the general relations

$$\begin{aligned}
&\hat{S}_z|s,m\rangle = m\hbar|s,m\rangle \\
&\hat{S}_\pm|s,m\rangle = \sqrt{s(s+1-m(m\pm 1)}\hbar|s,m\pm 1\rangle
\end{aligned}$$

7.7.48 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 $0 \le a \le 1$. 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

$$\hat{S}_+ |1,1\rangle = 0 \quad , \quad \hat{S}_+ |1,0\rangle = \sqrt{2}\,|1,1\rangle \quad , \quad \hat{S}_+ |1,-1\rangle = \sqrt{2}\,|1,0\rangle$$

it follows that

$$\langle\psi|\,\hat{S}_+\,|\psi\rangle = \sqrt{2}\,(x^*y + y^*z) \to x^*y = -y^*z$$

We also have

$$\langle\psi|\,\hat{S}_z\,|\psi\rangle = (x^*x - z^*z) = a = |x|^2 - |z|^2$$

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

$$\begin{array}{ll} |x|^2 - |z|^2 = a \quad , & |x|^2 + |z|^2 = 1 \\ |x|^2 = \frac{1+a}{2} \quad , & |z|^2 = \frac{1-a}{2} \end{array}$$

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 φ. In the special subcase $a = 1$, this reduces to the unique solution $|1,1\rangle$.

Case #2: The case $a = 0$ requires special treatment. Now $|y|$ need not vanish, and we find that, in general,

$$\left(|x|^2 - |z|^2\right)|y|^2 = 0 \to |x| = |z| = \alpha$$

If we fix the overall phase by requiring that y be real, then we have

$$x^*y = -y^*z = -yz \to x^* = -z$$

Now, the normalization condition gives

$$|x|^2 + |y|^2 + |z|^2 = 1 = 2\alpha^2 + y^2 \to y = \sqrt{1 - 2\alpha^2}$$

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, α and φ.

The above discussion applies to pure states.

More generally, a state can be expressed by an operator of the form

$$\hat{\rho} = \sum_{i=-1}^{1} \sum_{j=-1}^{1} \rho_{ij} \left|1, i\right\rangle \left\langle 1, j\right|$$

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.

7.7.49 Properties of an operator

An operator $\hat{f}$ describing the interaction of two spin$-1/2$ particles has the form $\hat{f} = a + b\vec{\sigma}_1 \cdot \vec{\sigma}_2$ where a and b are constants and $\vec{\sigma}_j = \sigma_{xj}\hat{\mathrm{x}} + \sigma_{yj}\hat{\mathrm{y}} + \sigma_{zj}\hat{\mathrm{z}}$ are Pauli matrix operators. The total spin angular momentum is

$$\vec{j} = \vec{j}_1 + \vec{j}_2 = \frac{\hbar}{2}\left(\vec{\sigma}_1 + \vec{\sigma}_2\right)$$

(a) Show that $\hat{f}$, $\vec{j}^2$ 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

$$\left[\hat{J}^2, \hat{J}_z\right] = 0 = \left[\hat{J}^2, a\right] = \left[\hat{J}_z, a\right]$$

Now

$$\hat{J}^2 = \frac{\hbar^2}{4}\left(\hat{\sigma}_1 + \hat{\sigma}_2\right)^2 = \frac{\hbar^2}{4}\left(\hat{\sigma}_1^2 + \hat{\sigma}_2^2 + 2\hat{\sigma}_1 \cdot \hat{\sigma}_2\right) \rightarrow \hat{\sigma}_1 \cdot \hat{\sigma}_2 = \frac{2}{\hbar^2}\hat{J}^2 - \frac{1}{2}\left(\hat{\sigma}_1^2 + \hat{\sigma}_2^2\right)$$

and

$$\hat{\sigma}_1^2 = \hat{\sigma}_2^2 = 3 \to \hat{\sigma}_1 \cdot \hat{\sigma}_2 = \frac{2}{\hbar^2}\hat{J}^2 - 3$$

Therefore,

$$\begin{aligned}
\left[\hat{J}^2, \hat{f}\right] &= \left[\hat{J}^2, a\right] + b\left[\hat{J}^2, \hat{\sigma}_1 \cdot \hat{\sigma}_2\right] = b\left[\hat{J}^2, \tfrac{2}{\hbar^2}\hat{J}^2 - 3\right] = 0 \\
\left[\hat{J}_z, \hat{f}\right] &= \left[\hat{J}_z, a\right] + b\left[\hat{J}_z, \hat{\sigma}_1 \cdot \hat{\sigma}_2\right] = b\left[\hat{J}_z, \tfrac{2}{\hbar^2}\hat{J}^2 - 3\right] = 0
\end{aligned}$$

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

$$\begin{aligned}
\langle J, M, j_1, j_2|\, \hat{f}\, |J', M', j_1, j_2\rangle &= a\delta_{JJ'}\delta_{MM'} + b\,\langle J, M, j_1, j_2| \left(\frac{2}{\hbar^2}\hat{J}^2 - 3\right)|J', M', j_1, j_2\rangle \\
&= \left(a + (2J(J+1) - 3)b\right)\delta_{JJ'}\delta_{MM'}
\end{aligned}$$

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 $|J, M, j_1, j_2\rangle \to |J, M\rangle$)

$$|0,0\rangle\ ,\ |1,1\rangle\ ,\ |1,0\rangle\ ,\ |1,-1\rangle$$

which give a diagonal matrix

$$f = \begin{pmatrix} a - 3b & 0 & 0 & 0 \\ 0 & a + b & 0 & 0 \\ 0 & 0 & a + b & 0 \\ 0 & 0 & 0 & a + b \end{pmatrix}$$

(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 $|j_1, j_2, m_1, m_2\rangle \to |m_1, m_2\rangle$) since j_1 and j_2 do not change. We then write

$$\begin{aligned}
\hat{f} &= a + b\hat{\sigma}_1 \cdot \hat{\sigma}_2 = a + b\left(\hat{\sigma}_{1x}\hat{\sigma}_{2x} + \hat{\sigma}_{1y}\hat{\sigma}_{2y} + \hat{\sigma}_{1z}\hat{\sigma}_{2z}\right) \\
&= a + b\left(\frac{\hat{\sigma}_{1+} + \hat{\sigma}_{1-}}{2}\frac{\hat{\sigma}_{2+} + \hat{\sigma}_{2-}}{2} + \frac{\hat{\sigma}_{1+} - \hat{\sigma}_{1-}}{2i}\frac{\hat{\sigma}_{2+} - \hat{\sigma}_{2-}}{2i} + \hat{\sigma}_{1z}\hat{\sigma}_{2z}\right) \\
&= a + b\left(\frac{\hat{\sigma}_{1+}\hat{\sigma}_{2-} + \hat{\sigma}_{1-}\hat{\sigma}_{2+}}{2} + \hat{\sigma}_{1z}\hat{\sigma}_{2z}\right)
\end{aligned}$$

The basis states are

$$\left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle \ , \ \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle \ , \ \left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle \ , \ \left|-\tfrac{1}{2},-\tfrac{1}{2}\right\rangle$$

and using

$$\begin{array}{l} \hat{\sigma}_+\left|\tfrac{1}{2}\right\rangle = 0 = \hat{\sigma}_-\left|-\tfrac{1}{2}\right\rangle \quad , \quad \hat{\sigma}_+\left|-\tfrac{1}{2}\right\rangle = 2\left|\tfrac{1}{2}\right\rangle \quad , \quad \hat{\sigma}_-\left|\tfrac{1}{2}\right\rangle = 2\left|-\tfrac{1}{2}\right\rangle \\ \hat{\sigma}_z\left|-\tfrac{1}{2}\right\rangle = -\left|-\tfrac{1}{2}\right\rangle \quad , \quad \hat{\sigma}_z\left|\tfrac{1}{2}\right\rangle = \left|\tfrac{1}{2}\right\rangle \end{array}$$

we have

$$\begin{array}{l} \hat{f}\left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle = (a+2b)\left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle \\ \hat{f}\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = a\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle + b\left(4\left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle - \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle\right) \\ \hat{f}\left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle = a\left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle + b\left(4\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle - \left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle\right) \\ \hat{f}\left|-\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = (a+2b)\left|-\tfrac{1}{2},-\tfrac{1}{2}\right\rangle \end{array}$$

Then

$$\begin{array}{l} \left\langle\tfrac{1}{2},\tfrac{1}{2}\right|\hat{f}\left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle = (a+2b)\left\langle\tfrac{1}{2},\tfrac{1}{2}\,\middle|\,\tfrac{1}{2},\tfrac{1}{2}\right\rangle = (a+2b) \\ \left\langle\tfrac{1}{2},-\tfrac{1}{2}\right|\hat{f}\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = a\left\langle\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle + b\left(4\left\langle\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,-\tfrac{1}{2},\tfrac{1}{2}\right\rangle - \left\langle\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle\right) = a-b \\ \left\langle\tfrac{1}{2},-\tfrac{1}{2}\right|\hat{f}\left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle = a\left\langle\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,-\tfrac{1}{2},\tfrac{1}{2}\right\rangle + b\left(4\left\langle\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle - \left\langle\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,-\tfrac{1}{2},\tfrac{1}{2}\right\rangle\right) = 4b \\ \left\langle\tfrac{1}{2},\tfrac{1}{2}\right|\hat{f}\left|-\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = (a+2b)\left\langle\tfrac{1}{2},\tfrac{1}{2}\,\middle|\,-\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = 0 \end{array}$$

so that

$$f = \begin{pmatrix} a+2b & 0 & 0 & 0 \\ 0 & a-b & 4b & 0 \\ 0 & 4b & a-b & 0 \\ 0 & 0 & 0 & a+2b \end{pmatrix}$$

7.7.50 Simple Tensor Operators/Operations

Given the tensor operator form of the particle coordinate operators

$$\vec{r} = (x,y,z);\ R_1^0 = z\ ,\ R_1^{\pm} = \mp\frac{x \pm iy}{\sqrt{2}}$$

(the subscript "1" indicates it is a rank 1 tensor), and the analogously defined particle momentum rank 1 tensor P_1^q, $q = 0, \pm 1$, calculate the commutator between each of the components and show that the results can be written in the form

$$[R_1^q, P_1^m] = \text{ simple expression}$$

We have

$$R_1^{\pm 1} = \mp\frac{R_x \pm iR_y}{\sqrt{2}} \quad , \quad P_1^{\pm 1} = \mp\frac{P_x \pm iP_y}{\sqrt{2}}$$

We can write (for generality)

$$R_1^q = -q\frac{R_x \pm qiR_y}{\sqrt{2}}\ ,\ etc$$

Now

$$\begin{aligned}
[R_1^q, P_1^m] &= \frac{1}{2}qm[R_x \pm qiR_y, P_x \pm miP_y] \\
&= \frac{1}{2}qm\left([R_x, P_x] + i^2qm[R_y, P_y]\right) = \frac{1}{2}qm(i\hbar) - \frac{1}{2}q^2m^2(i\hbar) \\
&= \frac{i\hbar}{2}[qm - 1] = \begin{cases} -i\hbar & q \neq m \\ 0 & q = m \end{cases}
\end{aligned}$$

So,

$$[R_1^q, P_1^m] = -i\hbar(1 - \delta_{qm}) = -i\hbar\delta_{q,-m}$$

Now,

$$[R_1^0, P_1^0] = [Z, P_z] = i\hbar$$

Clearly, R_1^0 commutes with $P_1^{\pm}$ and vice-versa.

A simple way to combine all of these results is

$$[R_1^q, P_1^m] = (-1)^q i\hbar\delta_{q,-m}$$

7.7.51 Rotations and Tensor Operators

Using the rank 1 tensor coordinate operator in Problem 9.7.50, calculate the commutators

$$[L_\pm, R_1^q] \text{ and } [L_z, R_1^q]$$

where $\vec{L}$ is the standard angular momentum operator.

We have

$$\begin{aligned}
[L_z, R_1^q] &= \left[L_z, -q\frac{R_x + iqR_y}{\sqrt{2}}\right] \\
&= -\frac{q}{\sqrt{2}}[L_z, R_x] - \frac{iq^2}{\sqrt{2}}[L_z, R_y] \\
&= -\frac{q}{\sqrt{2}}(i\hbar R_y) - \frac{i}{\sqrt{2}}(-i\hbar R_x) \\
&= -\frac{\hbar}{\sqrt{2}}(R_x + iqR_y) \\
&= q\hbar R_1^q
\end{aligned}$$

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

$$
\begin{aligned}
[L_\pm, R_1^q] &= [L_x \pm iL_y, R_1^q] \\
&= [L_x, R_1^q] \pm i[L_y, R_1^q] \\
&= \left[L_x, \frac{R_x + iqR_y}{\sqrt{2}}\right] \pm i\left[L_y, \frac{R_x + iqR_y}{\sqrt{2}}\right] \\
&= -\frac{q}{\sqrt{2}}[L_x, R_x] - \frac{i}{\sqrt{2}}[L_x, R_y] \pm i\left(-\frac{q}{\sqrt{2}}[L_y, R_x] - \frac{i}{\sqrt{2}}[L_y, R_y]\right) \\
&= 0 - \frac{i}{\sqrt{2}}(-zi\hbar) \pm i\left(0 - \frac{i}{\sqrt{2}}(-zi\hbar)\right) \\
&= -\frac{z\hbar}{\sqrt{2}} \pm \left(\frac{z\hbar}{\sqrt{2}}\right) \\
&= -\frac{\hbar}{\sqrt{2}} R_1^0 (1 \pm 1)
\end{aligned}
$$

So it should be $\pm\sqrt{2}\hbar R_1^0$, if it is nonzero. It means

$$
[L_+, R_1^1 = 0 = [L_-, R_1^{-1}] \quad , \quad [L_\pm, R_1^\mp] = \pm\sqrt{2}\hbar R_1^0
$$

7.7.52 Spin Projection Operators

Show that $\mathcal{P}_1 = \frac{3}{4}\hat{I} + (\vec{S}_1 \cdot \vec{S}_2)/\hbar^2$ and $\mathcal{P}_0 = \frac{1}{4}\hat{I} - (\vec{S}_1 \cdot \vec{S}_2)/\hbar^2$ project onto the spin-1 and spin-0 spaces in $\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$. Start by giving a mathematical statement of just what must be shown.

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

$$
\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\vec{S}^{\,2} - \vec{S}_1^2 - \vec{S}_2^2\right)
$$

where

$$
\begin{aligned}
\vec{S}_1^2 &= \hbar^2 S_1(S_1 + 1) = \frac{3\hbar^2}{4} \\
\vec{S}_2^2 &= \hbar^2 S_2(S_2 + 1) = \frac{3\hbar^2}{4}
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\mathcal{P}_1 &= \frac{3}{4}\hat{I} + (\vec{S}_1 \cdot \vec{S}_2)/\hbar^2 = \left(\frac{3}{4} + \frac{1}{2}S(S+1) - \frac{3}{4}\right)\hat{I} = \frac{1}{2}S(S+1)\hat{I} \\
\mathcal{P}_0 &= \frac{1}{4}\hat{I} - (\vec{S}_1 \cdot \vec{S}_2)/\hbar^2 = \left(\frac{3}{4} + \frac{1}{2}S(S+1) - \frac{3}{4}\right)\hat{I} = \left(1 - \frac{1}{2}S(S+1)\right)\hat{I}
\end{aligned}
$$

Then, clearly

$$\mathcal{P}_1 |1, M\rangle = \frac{1}{2}S(S+1)\hat{I} |1, M\rangle = |1, M\rangle$$

$$\mathcal{P}_1 |0, M\rangle = \frac{1}{2}S(S+1)\hat{I} |1, M\rangle = 0$$

$$\mathcal{P}_0 |1, M\rangle = \left(1 - \frac{1}{2}S(S+1)\right) \hat{I} |1, M\rangle = 0$$

$$\mathcal{P}_0 |0, M\rangle = \left(1 - \frac{1}{2}S(S+1)\right) \hat{I} |0, M\rangle = |0, M\rangle$$

which are the correct properties for the projection operators.

Note also that $\mathcal{P}_0 = 1 - \mathcal{P}_1$ or $\mathcal{P}_0 + \mathcal{P}_1 = 1$ and $\mathcal{P}_1^2 = \mathcal{P}_1$ and $\mathcal{P}_0^2 = \mathcal{P}_0$ which are also correct properties for projection operators.

7.7.53 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

$$H = A + \frac{J}{2\hbar^2}(S^2 - S_1^2 - S_2^2) + B\frac{S_z}{\hbar}$$

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

$$S = \frac{3}{2} \text{ with } M = \pm\frac{3}{2}, \pm\frac{1}{2}$$

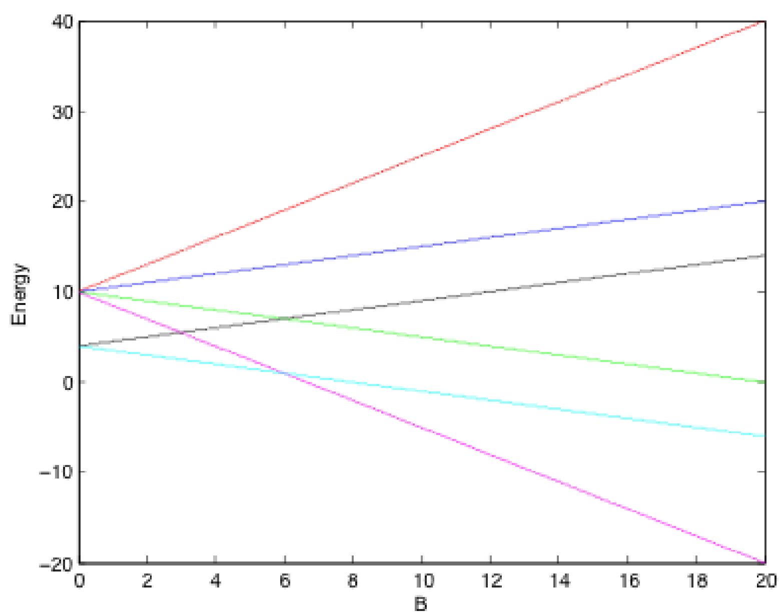
and

$$S = \frac{1}{2} \text{ with } M = \pm\frac{1}{2}$$

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:



7.7.54 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

$$|5/2, 1/2\rangle = \sqrt{\frac{2}{5}} |1, -1/2\rangle + \sqrt{\frac{3}{5}} |0, +1/2\rangle$$

Then, using orthogonality we get

$$|3/2, 1/2\rangle = \sqrt{\frac{3}{5}} |1, -1/2\rangle - \sqrt{\frac{2}{5}} |0, +1/2\rangle$$

7.7.55 The Rotation Operator for Spin$-1/2$

We learned that the operator

$$R_n(\Theta) = e^{-i\Theta(\vec{e}_n \cdot \hat{\mathbf{J}})/\hbar}$$

is a *rotation operator*, which rotates a vector about an axis $\vec{e}_n$ by and angle Θ. For the case of spin 1/2,

$$\hat{\mathbf{J}} = \hat{\mathbf{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}} \rightarrow R_n(\Theta) = e^{-i\Theta\hat{\sigma}_n/2}$$

(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

$$R_n(\Theta) = \sum_{m=0}^{\infty} \left(\frac{-i\Theta}{2}\right)^m \frac{(\hat{\sigma}_n)^m}{m!}$$

Now we have $(\hat{\sigma}_n)^2 = \hat{I}$, i.e, the square of any Pauli matrix is the identity matrix. Thus, we can separate the sum into even and odd terms

$$(\hat{\sigma}_n)^m = \begin{cases} \hat{I} & m \text{ even} \\ \hat{\sigma}_n & m \text{ odd} \end{cases}$$

Moreover,

$$(-i)^m = \begin{cases} (-1)^{m/2} & m \text{ even} \\ -i(-1)^{(m-1)/2} & m \text{ odd} \end{cases}$$

This implies that

$$R_n(\Theta) = \left(\sum_{m\ even} (-1)^{m/2} \left(\frac{\Theta}{2}\right)^m \frac{1}{m!}\right) \hat{I} - i \left(\sum_{m\ odd} (-1)^{(m-1)/2} \left(\frac{\Theta}{2}\right)^m \frac{1}{m!}\right) \hat{\sigma}_n$$

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,

$$R_n(\Theta = 2\pi)\left|\psi\right\rangle = -\left|\psi\right\rangle$$

For any $|psi\rangle$ describing a spin$-1/2$ state, this is the famous phase associayed with spinors, that differentiates it from orbital angular momentum.

(c) Consider a series of rotations. Rotate about the $y-$axis by θ followed by a rotation about the $z-$axis by ϕ. Convince yourself that this takes the unit vector along $\vec{e}_z$ to $\vec{e}_n$. Show that up to an overall phase

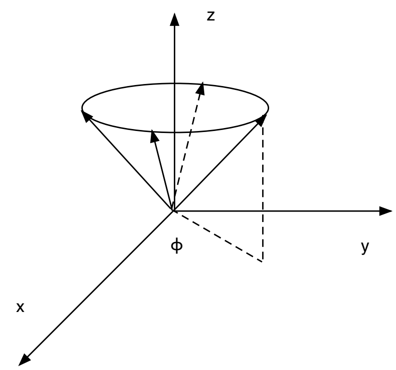
$$\left|\uparrow_n\right\rangle = R_z(\phi)R_y\left|\uparrow_z\right\rangle$$

We obtain a vector in the (θ, ϕ) direction by first rotating about the $y-$axis by θ and then about the the $z-$axis by ϕ. We have

$$\hat{R}_y(\theta) = \cos\frac{\theta}{2}\hat{I} - i\sin\frac{\theta}{2}\hat{\sigma}_y$$

In the $\{\left|\uparrow_z\right\rangle, \left|\downarrow_z\right\rangle\}$ basis we have

$$\hat{R}_y(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$



Therefore,

$$\hat{R}_y(\theta)\left|\uparrow_z\right\rangle = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}$$

Now follow this by a rotation about the $z-$axis by ϕ where

$$\hat{R}_z(\phi) = \cos\frac{\phi}{2}\hat{I} - i\sin\frac{\phi}{2}\hat{\sigma}_z$$

Again, in the $\{\left|\uparrow_z\right\rangle, \left|\downarrow_z\right\rangle\}$ basis we have

$$\hat{R}_z(\phi) = \begin{pmatrix} \cos\frac{\phi}{2} - i\sin\frac{\phi}{2} & 0 \\ 0 & \cos\frac{\theta}{2} + i\sin\frac{\phi}{2} \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{+i\frac{\phi}{2}} \end{pmatrix}$$

Therefore,

$$\hat{R}_z(\phi)\left(\hat{R}_y(\theta)\left|\uparrow_z\right\rangle\right) = \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{+i\frac{\phi}{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ e^{+i\frac{\phi}{2}}\sin\frac{\theta}{2} \end{pmatrix}$$

Therefore,

$$\hat{R}_z(\phi)\left(\hat{R}_y(\theta)\left|\uparrow_z\right\rangle\right) = e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2}\left|\uparrow_z\right\rangle + e^{+i\frac{\phi}{2}}\sin\frac{\theta}{2}\left|\downarrow_z\right\rangle$$

or neglecting an overall phase factor

$$\hat{R}_z(\phi)\left(\hat{R}_y(\theta)\left|\uparrow_z\right\rangle\right) = \cos\frac{\theta}{2}\left|\uparrow_z\right\rangle + e^{+i\phi}\sin\frac{\theta}{2}\left|\downarrow_z\right\rangle$$

so that

$$\hat{R}_z(\phi)\left(\hat{R}_y(\theta)\left|\uparrow_z\right\rangle\right) = \left|\uparrow_n\right\rangle$$

7.7.56 The Spin Singlet

Consider the entangled state of two spins

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle_A \otimes |\downarrow_z\rangle_B - |\downarrow_z\rangle_A \otimes |\uparrow_z\rangle_B\right)$$

(a) Show that (up to a phase)

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_n\rangle_A \otimes |\downarrow_n\rangle_B - |\downarrow_n\rangle_A \otimes |\uparrow_n\rangle_B\right)$$

where $|\uparrow_n\rangle$, $|\downarrow_n\rangle$ are spin spin-up and spin-down states along the direction $\vec{e}_n$. Interpret this result.

We have

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle_A \otimes |\downarrow_z\rangle_B - |\downarrow_z\rangle_A \otimes |\uparrow_z\rangle_B\right)$$

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

$$\begin{aligned}|\uparrow_n\rangle &= \cos\tfrac{\theta}{2}|\uparrow_z\rangle + e^{+i\phi}\sin\tfrac{\theta}{2}|\downarrow_z\rangle \\ |\downarrow_n\rangle &= \sin\tfrac{\theta}{2}|\uparrow_z\rangle - e^{+i\phi}\cos\tfrac{\theta}{2}|\downarrow_z\rangle\end{aligned}$$

are the spin-up and spin-down states along an arbitrary quantization axis defined by polar angles (θ, ϕ).

Consider then

$$\begin{aligned}
&\frac{1}{\sqrt{2}}\left(|\uparrow_n\rangle|\downarrow_n\rangle - |\downarrow_n\rangle|\uparrow_n\rangle\right) \\
&= \frac{1}{\sqrt{2}}\left((\cos\frac{\theta}{2}|\uparrow_z\rangle + e^{+i\phi}\sin\frac{\theta}{2}|\downarrow_z\rangle)\otimes(\sin\frac{\theta}{2}|\uparrow_z\rangle - e^{+i\phi}\cos\frac{\theta}{2}|\downarrow_z\rangle)\right) \\
&\quad - \frac{1}{\sqrt{2}}\left((\sin\frac{\theta}{2}|\uparrow_z\rangle - e^{+i\phi}\cos\frac{\theta}{2}|\downarrow_z\rangle)\otimes(\cos\frac{\theta}{2}|\uparrow_z\rangle + e^{+i\phi}\sin\frac{\theta}{2}|\downarrow_z\rangle)\right) \\
&= -\frac{e^{+i\phi}}{\sqrt{2}}\left((\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2})|\uparrow_z\rangle|\downarrow_z\rangle - (\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2})|\downarrow_z\rangle|\uparrow_z\rangle\right) \\
&= -e^{+i\phi}|\Psi_{AB}\rangle
\end{aligned}$$

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

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle \otimes |\downarrow_z\rangle - |\downarrow_z\rangle \otimes |\uparrow_z\rangle\right)$$

which implies that

$$\hat{\sigma}_n \otimes \hat{\sigma}_{n'} |\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} \left(\hat{\sigma}_n |\uparrow_z\rangle \otimes \hat{\sigma}_{n'} |\downarrow_z\rangle - \hat{\sigma}_n |\downarrow_z\rangle \otimes \hat{\sigma}_{n'} |\uparrow_z\rangle\right)$$

Thus,

$$\begin{aligned}
&\langle\Psi_{AB}| \hat{\sigma}_n \otimes \hat{\sigma}_{n'} |\Psi_{AB}\rangle \\
&\quad = \frac{1}{2} \langle\uparrow_z| \hat{\sigma}_n |\uparrow_z\rangle \langle\downarrow_z| \hat{\sigma}_{n'} |\downarrow_z\rangle - \frac{1}{2} \langle\downarrow_z| \hat{\sigma}_n |\uparrow_z\rangle \langle\uparrow_z| \hat{\sigma}_{n'} |\downarrow_z\rangle \\
&\quad - \frac{1}{2} \langle\uparrow_z| \hat{\sigma}_n |\downarrow_z\rangle \langle\downarrow_z| \hat{\sigma}_{n'} |\uparrow_z\rangle + \frac{1}{2} \langle\downarrow_z| \hat{\sigma}_n |\downarrow_z\rangle \langle\uparrow_z| \hat{\sigma}_{n'} |\uparrow_z\rangle
\end{aligned}$$

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,

$$\begin{aligned}
&\langle\Psi_{AB}| \hat{\sigma}_n \otimes \hat{\sigma}_{n'} |\Psi_{AB}\rangle \\
&\quad = \frac{1}{2} \left(-\cos\theta\cos\theta' - e^{i(\phi-\phi')}\sin\theta\sin\theta'\right) \\
&\quad\quad - \left(-e^{-i(\phi-\phi')}\sin\theta\sin\theta' - \cos\theta\cos\theta'\right) \\
&\quad = -\left(\cos\theta\cos\theta' + \cos\left(\phi-\phi'\right)\sin\theta\sin\theta'\right)
\end{aligned}$$

Now

$$\begin{aligned}
\vec{e}_n &= \cos\theta\vec{e}_z + \sin\theta(\cos\phi\vec{e}_x + \sin\phi\vec{e}_y) \\
\vec{e}_{n'} &= \cos\theta'\vec{e}_z + \sin\theta'(\cos\phi'\vec{e}_x + \sin\phi'\vec{e}_y)
\end{aligned}$$

so that

$$\begin{aligned}
\vec{e}_n \cdot \vec{e}_{n'} &= \cos\theta\cos\theta' + \sin\theta\sin\theta'(\cos\phi\cos\phi' + \sin\phi\sin\phi') \\
&= \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos\left(\phi-\phi'\right)
\end{aligned}$$

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.

7.7.57 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

$$a = \frac{\hbar^2}{me^2} \quad , \quad E = -\frac{\hbar^2}{2ma^2\alpha^2} \quad , \quad z = \frac{2x}{\alpha a}$$

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

$$\begin{aligned}
&\psi(x,y,z) = \psi_n(x)\varphi_y(y)\varphi_z(z)\\
&-\tfrac{\hbar^2}{2m}\tfrac{d^2\psi_n(x)}{dx^2} - \tfrac{e^2}{x}\psi_n(x) = E_x\psi_n(x)\\
&-\tfrac{\hbar^2}{2m}\tfrac{d^2\varphi_y(y)}{dy^2} = \tfrac{p_y^2}{2m}\varphi_y(y) \quad , \quad -\tfrac{\hbar^2}{2m}\tfrac{d^2\varphi_z(z)}{dz^2} = \tfrac{p_z^2}{2m}\varphi_z(z)\\
&E = \tfrac{p_y^2}{2m} + \tfrac{p_z^2}{2m} + E_x = E_x
\end{aligned}$$

since confinement to the $x-$axis means that $p_y = p_z = 0$. This leaves us with the equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} - \frac{e^2}{x}\psi_n(x) = E_x\psi_n(x)$$

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

$$r \to x \quad , \quad Z = 1$$

Therefore, the ground state solution is

$$\psi_1(x) = xR_{10}(x) = 2x\left(\frac{1}{a}\right)^{3/2} e^{-x/a} \quad , \quad a = \frac{\hbar^2}{me^2}$$

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.

7.7.58 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 ℓ quantum number for this electron?

The general solution for the Schrodinger equation of the hydrogen atom is

$$\psi(r,\theta,\phi) = NR_{n\ell}(r)Y_{\ell m}(\theta,\phi)$$

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

$$\begin{aligned}
\hat{L}^2\psi_{p_z} &= \hat{L}^2\sqrt{\frac{3}{4\pi}} R_{n\ell}(r)\cos\theta \\
&= -\sqrt{\frac{3}{4\pi}} R_{n\ell}(r)\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\cos\theta \\
&= -\sqrt{\frac{3}{4\pi}} R_{n\ell}(r)\hbar^2 \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial(cos\theta)}{\partial\theta}\right) \\
&- \sqrt{\frac{3}{4\pi}} R_{n\ell}(r)\hbar^2 \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin^2\theta) \\
&= 2\hbar^2\sqrt{\frac{3}{4\pi}} R_{n\ell}(r)cos\theta = 2\hbar^2\psi_{p_z}
\end{aligned}$$

(b) In general, for an electron with this ℓ quantum number, what are the allowed values of m_ℓ? (NOTE: you should not restrict yourself to a p_z electron here). What are the allowed values of s and m_s?

$m = m_\ell$ can always take the values $-\ell, -\ell+1, ..., +\ell$. 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_ℓ values for a single electron in a $p-$orbital. Given the Clebsch-Gordon coefficients shown in the table below

					$\|j, m_j\rangle$		
m_{j_1}	m_{j_2}	$\|3/2, 3/2\rangle$	$\|3/2, 1/2\rangle$	$\|1/2, 1/2\rangle$	$\|3/2, -1/2\rangle$	$\|1/2, -1/2\rangle$	$\|3/2, -3/2\rangle$
1	1/2	1					
1	-1/2		$\sqrt{1/3}$	$\sqrt{2/3}$			
0	1/2		$\sqrt{2/3}$	$-\sqrt{1/3}$			
0	-1/2				$\sqrt{2/3}$	$\sqrt{1/3}$	
-1	1/2				$\sqrt{1/3}$	$-\sqrt{2/3}$	
-1	-1/2						1

Table 7.1: 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_ℓ, m_s are allowed:

m_ℓ	m_s
1	1/2
1	-1/2
0	1/2
0	-1/2
-1	1/2
-1	-1/2

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, $\hat{H}_{so}$ is given by

$$\hat{H}_{so} = \xi(\vec{r})\hat{\ell} \cdot \hat{s}$$

Show that the states with $|j, m_j\rangle$ equal to $|3/2, 3/2\rangle$, $|3/2, 1/2\rangle$ and $|1/2, 1/2\rangle$ are eigenstates of the spin-orbit coupling Hamiltonian and find the corresponding eigenvalues. Comment on which quantum numbers determine the spin-orbit energy. (HINT: there is a rather quick and easy way to do this, so if you are doing something long and tedious you might want to think again .....).

There are two ways to approach this part.

First Method: We write

$$\hat{H}_{so} = \xi(\vec{r})\hat{\ell} \cdot \hat{s} = \xi(\vec{r})\left(\hat{\ell}_z\hat{s}_z + \frac{1}{2}(\hat{\ell}_+\hat{s}_- + \hat{\ell}_-\hat{s}_+\right)$$

Then, operating on the $|j, m_j\rangle$ states written in the $|m+\ell, m_s\rangle$ basis, we get

$$\begin{aligned}\hat{H}_{so}|3/2,3/2\rangle &= \xi(\vec{r})\left(\hat{\ell}_z\hat{s}_z + \frac{1}{2}(\hat{\ell}_+\hat{s}_- + \hat{\ell}_-\hat{s}_+\right)|1,1/2\rangle \\ &= \xi(\vec{r})(\hbar)(\hbar/2)|1,1/2\rangle = \frac{\hbar^2}{2}\xi(\vec{r})|3/2,3/2\rangle\end{aligned}$$

Thus, the state $|3/2,3/2\rangle$ is an eigenstates of $\hat{H}_{so}$ with eigenvalue $\hbar^2\xi(\vec{r})/2$.

Continuing we have

$$\begin{aligned}\hat{H}_{so}|3/2,1/2\rangle &= \xi(\vec{r})\left(\hat{\ell}_z\hat{s}_z + \frac{1}{2}(\hat{\ell}_+\hat{s}_- + \hat{\ell}_-\hat{s}_+\right)(\sqrt{2/3}|0,1/2\rangle + \sqrt{1/3}|1,-1/2\rangle) \\ &= \xi(\vec{r})\left(\hat{\ell}_z\hat{s}_z + \frac{1}{2}(\hat{\ell}_+\hat{s}_- + \hat{\ell}_-\hat{s}_+\right)\sqrt{2/3}|0,1/2\rangle \\ &\quad + \xi(\vec{r})\left(\hat{\ell}_z\hat{s}_z + \frac{1}{2}(\hat{\ell}_+\hat{s}_- + \hat{\ell}_-\hat{s}_+\right)\sqrt{1/3}|1,-1/2\rangle \\ &= \frac{\hbar^2}{2}\xi(\vec{r})(\sqrt{2/3}|0,1/2\rangle + \sqrt{1/3}|1,-1/2\rangle) = \frac{\hbar^2}{2}\xi(\vec{r})|3/2,1/2\rangle\end{aligned}$$

Thus, the state $|3/2,1/2\rangle$ is an eigenstates of $\hat{H}_{so}$ 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 $\hat{H}_{so}$ with eigenvalue $\hbar^2\xi(\vec{r})/2$.

Finally,

$$\begin{aligned}\hat{H}_{so}|1/2,1/2\rangle &= \xi(\vec{r})\left(\hat{\ell}_z\hat{s}_z + \frac{1}{2}(\hat{\ell}_+\hat{s}_- + \hat{\ell}_-\hat{s}_+\right)(-\sqrt{1/3}|0,1/2\rangle + \sqrt{2/3}|1,-1/2\rangle) \\ &= -\hbar^2\xi(\vec{r})(-\sqrt{1/3}|0,1/2\rangle + \sqrt{2/3}|1,-1/2\rangle) = -\hbar^2\xi(\vec{r})|1/2,1/2\rangle\end{aligned}$$

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

$$\hat{j}^2 = (\hat{\ell} + \hat{s})^2 = \hat{\ell}^2 + \hat{s}^2 + 2\hat{\ell}\cdot\hat{s}$$

so that

$$\hat{\ell}\cdot\hat{s} = \frac{1}{2}(\hat{j}^2 - \hat{\ell}^2 - \hat{s}^2)$$

Then, since all the states have simultaneously well-defined values of j, ℓ, and s, they are all eigenstates of $\hat{j}^2$, $\hat{\ell}^2$, and $\hat{s}^2$ and hence of $\hat{H}_{so}$. To find the eigenvalues we just operate on a general state

$$\begin{aligned}
\hat{H}_{so}\,|j,m_j\rangle &= \frac{\xi(\vec{r})}{2}(\hat{j}^2-\hat{\ell}^2-\hat{s}^2)\,|j,m_j\rangle \\
&= \frac{\hbar^2\xi(\vec{r})}{2}(j(j+1)-\ell(\ell+1)-s(s+1))\,|j,m_j\rangle \\
&= \frac{\hbar^2\xi(\vec{r})}{2}(j(j+1)-11/4)\,|j,m_j\rangle \qquad (7.7)
\end{aligned}$$

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 ℓ and s), i.e., it depends on how ℓ 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

$$R_{n\ell}(r) = \left(\frac{Z}{a_0}\right)^{3/2}\frac{1}{2\sqrt{6}}\rho e^{-\rho/2}$$

(where $\rho = Zr/a_0$ and $a_0 = 4\pi\varepsilon_0\hbar^2/m_e c^2$) derive an expression for the spin-orbit coupling constant for an electron in a $2p-$orbital. Comment on the dependence on the atomic number Z.

We need to calculate

$$\begin{aligned}
\int_0^\infty \xi(r)|R_{21}(r)|^2 r^2 dr &= \frac{Ze^2}{8\pi\varepsilon_0 m_e^2 c^2}\int_0^\infty \frac{1}{r^3}|R_{21}(r)|^2 r^2 dr \\
&= \frac{Ze^2}{8\pi\varepsilon_0 m_e^2 c^2}\frac{1}{24}\left(\frac{Z}{a_0}\right)^5\int_0^\infty r e^{-Zr/a_0} dr \\
&= \frac{Ze^2}{8\pi\varepsilon_0 m_e^2 c^2}\frac{1}{24}\left(\frac{Z}{a_0}\right)^3 \\
&= \frac{m_e e^8}{1536\varepsilon_0^3 c^2 \pi\hbar^6}Z^4
\end{aligned}$$

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

$$\hat{H}^{(1)} = \mu_B B(\hat{\ell}_z + 2\hat{s}_z)$$

The change in energy due to a small perturbation is given in first-order perturbation theory by

$$E^{(1)} = \langle 0| \hat{H}^{(1)} |0\rangle$$

where $|0\rangle$ is the unperturbed state (i.e., in this example, the state in the absence of the applied field). Use this expression to show that the change in the energies of the states in part (d) is described by

$$E^{(1)} = \mu_B B g_j m_j \tag{7.8}$$

and find the values of g_j. We will prove the perturbation theory result in the Chapter 10.

We have

$$E^(1) = \langle j, m_j| \mu_B B(\hat{\ell}_z + 2\hat{s}_z) |j, m_j\rangle$$

To do the calculation, we rewrite the $|j, m_j\rangle$ states in the $|m_\ell, m_s\rangle$ basis. Then we have for $|j, m_j\rangle = |3/2, 3/2\rangle = |1, 1/2\rangle$

$$\begin{aligned} E^(1) &= \langle 1, 1/2| \mu_B B(\hat{\ell}_z + 2\hat{s}_z) |1, 1/2\rangle = 2\hbar\mu_B B \\ &= \mu_B B \frac{4}{3}\hbar m_j = \mu_B B g_j \hbar m_j \text{ with } g_j = \frac{4}{3}\hbar \end{aligned}$$

Similarly, we have for $|j, m_j\rangle = |3/2, 1/2\rangle = \sqrt{\frac{2}{3}}\,|0, 1/2\rangle + \sqrt{\frac{1}{3}}\,|1, -1/2\rangle$

$$\begin{aligned} E^(1) &= \mu_B B\left(\frac{2}{3}\langle 0, 1/2| \hat{\ell}_z + 2\hat{s}_z |0, 1/2\rangle + \frac{1}{3}\langle 1, -1/2| \hat{\ell}_z + 2\hat{s}_z |1, -1/2\rangle\right) \\ &= \mu_B B\left(\frac{2}{3}\hbar + \frac{1}{3}(0)\right) = \mu_B B \frac{4}{3}\hbar m_j = \mu_B B g_j m_j \text{ with } g_j = \frac{4}{3}\hbar \end{aligned}$$

Similarly, we get for $|j, m_j\rangle = |1/2, 1/2\rangle = \sqrt{\frac{1}{3}}\,|0, 1/2\rangle + \sqrt{\frac{2}{3}}\,|1, -1/2\rangle$

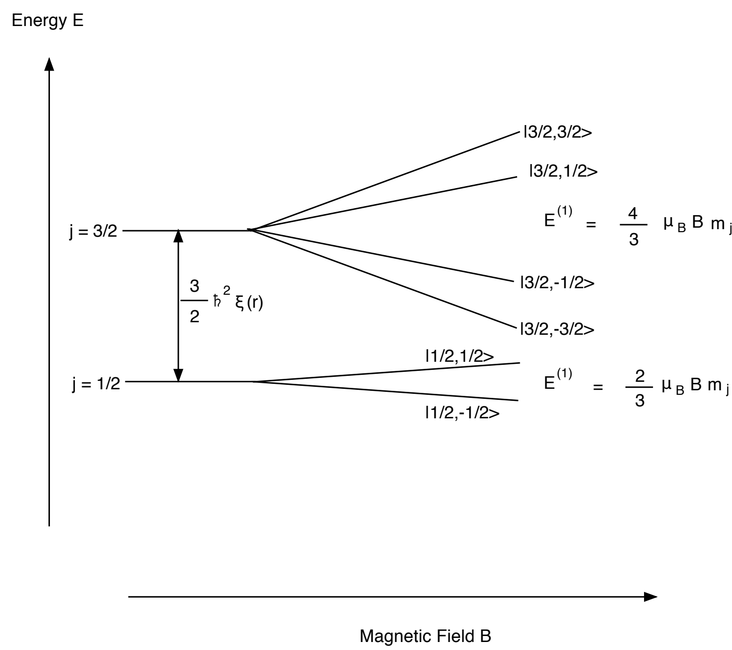
$$E^(1) = \mu_B B g_j m_j \text{ with } g_j = \frac{2}{3}\hbar$$

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.

7.7.59 Quadrupole Moment Operators

The quadrupole moment operators can be written as

$$\begin{aligned}
Q^{(+2)} &= \sqrt{\frac{3}{8}}(x+iy)^2 \\
Q^{(+1)} &= -\sqrt{\frac{3}{2}}(x+iy)z \\
Q^{(0)} &= \frac{1}{2}(3z^2 - r^2) \\
Q^{(-1)} &= \sqrt{\frac{3}{2}}(x-iy)z \\
Q^{(-2)} &= \sqrt{\frac{3}{8}}(x-iy)^2
\end{aligned}$$

Using the form of the wave function $\psi_{\ell m} = R(r)Y_m^\ell(\theta, \phi)$,

(a) Calculate $\langle \psi_{3,3} | Q^{(0)} | \psi_{3,3} \rangle$

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

$$\frac{Q_0}{r^2} = \frac{1}{2r^2}(3z^2 - r^2) = \frac{1}{2}(3\cos^2\theta - 1)$$

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:

```
q0 = 1/2 (3 Cos[θ]^2 - 1);
shavg[m2_, q_, m1_] := Integrate[Conjugate[SphericalHarmonicY[3, m2, θ, ϕ]]
    q SphericalHarmonicY[3, m1, θ, ϕ] Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}];
```

and then compute

(b) Predict all others $\langle \psi_{3,m'} | Q^{(0)} | \psi_{3,m} \rangle$ using the Wigner-Eckart theorem in terms of Clebsch-Gordon coefficients.

Using the result above, the double-bar-inner-product on the RHS of the

```
q0a33 = shavg[3, q0, 3]
```

$-\frac{1}{3}$

```
dbavg = q0a33 / ClebschGordan[{3, 3}, {2, 0}, {3, 3}] * √7
```

$-2\sqrt{\frac{7}{15}}$

```
weavg[m2_, q_, m1_] := ClebschGordan[{3, m1}, {2, q}, {3, m2}] * dbavg / √7 ;
```

Wigner-Eckhart theorem is
Then, we can insert this in a general function for any m_1 and m_2:
or written out...

$$\langle 3, m_2|\,(Q^{(2)})_q\,|3, m_1\rangle = \left(\frac{1}{\sqrt{7}}\right)\langle 3, 2; m_1, q\,|\,3, 2 : 3, m_2\rangle\left(-2\sqrt{\frac{7}{15}}\right)$$

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 $m_1 + q = m_2$ amd $|j_1 - j_2| < k < j_1 + j_2$, 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):
and compute the inner products using the *shavg* function from (a);

Note that we leave $\langle r^2\rangle = \int_0^\infty r^2\,dr R^2(r) r^2$ as an overall constant that drops out from the ratios.

```
qp1 = -Sqrt[3/2] (Sin[θ] Cos[ϕ] + I Sin[θ] Sin[ϕ]) Cos[θ];
qm2 = Sqrt[3/8] (Sin[θ] Cos[ϕ] - I Sin[θ] Sin[ϕ])^2;
```

```
shavg[1, qp1, 0]
shavg[-1, qm2, 1]
shavg[-2, q0, -3]
```

$$\frac{\sqrt{2}}{15}$$

$$-\frac{2\sqrt{\frac{2}{3}}}{5}$$

$$0$$

Compare the results using the Wigner-Eckhart function from (b):

```
weavg[1, 1, 0]
weavg[-1, -2, 1]
weavg[-2, 0, -3]
```

$$\frac{\sqrt{2}}{15}$$

$$-\frac{2\sqrt{\frac{2}{3}}}{5}$$

```
ClebschGordan::phy : ThreeJSymbol[{3, -3}, {2, 0}, {3, 2}] is not physical. More...
```

$$0$$

7.7.60 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

$$J_{\pm}\,|j_1j_2;jm\rangle = (J_{1\pm}+J_{2\pm})\sum_{m_1}\sum_{m_2}|j_1j_2;m_1m_2\rangle\,\langle j_1j_2;m_1m_2\,|\,j_1j_2;jm\rangle$$

where

$$C(j_1j_2j;m_1m_2m) = \langle j_1j_2;m_2m_2\,|\,j_1j_2;jm\rangle = \text{ Clebsch-Gordon coefficient}$$

Expanding out we have

$$\begin{aligned}
&\sqrt{(j\mp m)(j\pm m+1)}\,|j_1j_2;jm\pm 1\rangle \\
&\quad=\sum_{m_1'}\sum_{m_2'}\sqrt{(j_1\mp m_1')(j_1\pm m_1'+1)}\,|j_1j_2;m_1'\pm 1,m_2'\rangle\,\langle j_1j_2;m_1'm_2'\,|\,j_1j_2;jm\rangle \\
&\quad+\sum_{m_1'}\sum_{m_2'}\sqrt{(j_2\mp m_2')(j_2\pm m_2'+1)}\,|j_1j_2;m_1',m_2'\pm 1\rangle\,\langle j_1j_2;m_1'm_2'\,|\,j_1j_2;jm\rangle
\end{aligned}$$

Using orthonormality, we take the scalar product with $\langle j_1j_2;m_1m_2|$ 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:

$$\begin{aligned}
&\sqrt{(j\mp m)(j\pm m+1)}C(j_1j_2j;m_1,m_2,m\pm 1) \\
&\quad=\sqrt{(j_1\mp m_1+1)(j_1\pm m_1)}C(j_1j_2j;m_1\mp 1,m_2,m) \\
&\quad+\sqrt{(j_2\mp m_2+1)(j_2\pm m_2)}C(j_1j_2j;m_1,m_2\mp 1,m)
\end{aligned}$$

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

$$C(3/2,1,5/2;3/2,0,3/2) = \sqrt{\frac{2}{5}}$$

and

$$\sqrt{5}C(3/2,1,5/2;1/2,1,3/2) = \sqrt{3}C(3/2,1,5/2;3/2,1,5/2)$$

so that

$$C(3/2,1,5/2;1/2,1,3/2) = \sqrt{\frac{3}{5}}$$

and therefore

$$\begin{aligned}
|3/21;5/2,3/2\rangle &= C(3/2,1,5/2;1/2,1,3/2)\,|3/2,1;1/2,1\rangle \\
&\quad + C(3/2,1,5/2;3/2,0,3/2)\,|3/2,1;3/2,0\rangle
\end{aligned}$$

```
lower[j_, m_] = √((j + m) (j - m + 1));
```

or

$$|3/21;5/2,3/2\rangle = \sqrt{\frac{3}{5}}\,|3/2,1;1/2,1\rangle + \sqrt{\frac{2}{5}}\,|3/2,1;3/2,0\rangle$$

This leads to the following sequence using Mathematica. We implement the lowering eigenvalue
Then we start from the maximum state($j = 5/2, m = 5/2$) and write for $m = 3/2$:

```
lower[3 / 2, 3 / 2] / lower[5 / 2, 5 / 2]
lower[1, 1] / lower[5 / 2, 5 / 2]
```

$$\sqrt{\frac{3}{5}}$$

$$\sqrt{\frac{2}{5}}$$

Thus we get (as before)

$$C(3/2,1,5/2;1/2,1,3/2) = \sqrt{\frac{3}{5}}$$
$$C(3/2,1,5/2;3/2,0,3/2) = \sqrt{\frac{2}{5}}$$

Then for $m = 1/2$:

```
√3/5 lower[3/2, 1/2]/lower[5/2, 3/2]
√3/5 lower[1, 1]/lower[5/2, 3/2]

√2/5 lower[3/2, 3/2]/lower[5/2, 3/2]
√2/5 lower[1, 0]/lower[5/2, 3/2]
```

$$\sqrt{\frac{3}{10}}$$

$$\frac{\sqrt{\frac{3}{5}}}{2}$$

$$\frac{\sqrt{\frac{3}{5}}}{2}$$

$$\frac{1}{\sqrt{10}}$$

so that we get

$$C(3/2,1,5/2;-1/2,1,1/2) = \sqrt{\frac{3}{10}}$$
$$C(3/2,1,5/2;1/2,0,1/2) = \frac{1}{2}\sqrt{\frac{3}{5}} + \frac{1}{2}\sqrt{\frac{3}{5}} = \sqrt{\frac{3}{5}}$$
$$C(3/2,1,5/2;3/2,-1,1/2) = \sqrt{\frac{1}{10}}$$

Note that the second and third terms end up as $|3/2,1/2\rangle \otimes |1,0\rangle$ and we just add their contributions.

Then for $m = -1/2$:
so that

$$C(3/2,1,5/2;-3/2,1,-1/2) = \sqrt{\frac{1}{10}}$$
$$C(3/2,1,5/2;-1/2,0,-1/2) = \sqrt{\frac{1}{15}} + 2\sqrt{\frac{1}{15}} = \sqrt{\frac{3}{5}}$$
$$C(3/2,1,5/2;1/2,-1,-1/2) = \sqrt{\frac{2}{15}} + \sqrt{\frac{1}{30}} = \sqrt{\frac{3}{10}}$$

```
√3 / 10 lower[3 / 2, -1 / 2] / lower[5 / 2, 1 / 2]
√3 / 10 lower[1, 1] / lower[5 / 2, 1 / 2]

√3 / 5 lower[3 / 2, 1 / 2] / lower[5 / 2, 1 / 2]
√3 / 5 lower[1, 0] / lower[5 / 2, 1 / 2]

√1 / 10 lower[3 / 2, 3 / 2] / lower[5 / 2, 1 / 2]
```

$$\frac{1}{\sqrt{10}}$$

$$\frac{1}{\sqrt{15}}$$

$$\frac{2}{\sqrt{15}}$$

$$\sqrt{\frac{2}{15}}$$

$$\frac{1}{\sqrt{30}}$$

Note that we omitted the term which would have lowered $|1, -1\rangle$.

Then for $m = -3/2$:

```
√1 / 10 lower[1, 1] / lower[5 / 2, -1 / 2]

√3 / 5 lower[3 / 2, -1 / 2] / lower[5 / 2, -1 / 2]
√3 / 5 lower[1, 0] / lower[5 / 2, -1 / 2]

√3 / 10 lower[3 / 2, 1 / 2] / lower[5 / 2, -1 / 2]
```

$$\frac{1}{2\sqrt{10}}$$

$$\frac{3}{2\sqrt{10}}$$

$$\frac{\sqrt{\frac{3}{5}}}{2}$$

$$\frac{\sqrt{\frac{3}{5}}}{2}$$

so that

$$C(3/2, 1, 5/2; -3/2, 0, -3/2) = \frac{1}{2}\sqrt{\frac{1}{10}} + \frac{1}{2}\sqrt{\frac{9}{10}} = \sqrt{\frac{2}{5}}$$
$$C(3/2, 1, 5/2; 1/2, -1, -1/2) = \frac{1}{2}\sqrt{\frac{3}{5}} + \frac{1}{2}\sqrt{\frac{3}{5}} = \sqrt{\frac{3}{5}}$$

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 $m = -5/2$:

```
√(2/5) lower[1, 0] / lower[5/2, -3/2]
√(3/5) lower[3/2, -1/2] / lower[5/2, -3/2]
```

$$\frac{2}{5}$$

$$\frac{3}{5}$$

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 $|j_1 m_1\rangle \otimes |j_2 m_2\rangle$ is equal to the number of irreducible representations.

Knowing this, we can immediately write down the the CG coefficients for the maimum m state of the sum representation $j = 3/2$, $|3/3, 3/2\rangle$:

$$C(3/2,1,3/2;1/2,1,3/2) = -\sqrt{\frac{2}{5}}$$

$$C(3/2,1,3/2;3/2,0,3/2) = \sqrt{\frac{3}{5}}$$

Note that we have fixed a sign convention.

We can now proceed in the same fashion as before. First, for $m = 1/2$:

```
-√2/5 lower[3/2, 1/2] / lower[3/2, 3/2]
-√2/5 lower[1, 1] / lower[3/2, 3/2]

√3/5 lower[3/2, 3/2] / lower[3/2, 3/2]
√3/5 lower[1, 0] / lower[3/2, 3/2]
```

$-2\sqrt{\frac{2}{15}}$

$-\frac{2}{\sqrt{15}}$

$\sqrt{\frac{3}{5}}$

$\sqrt{\frac{2}{5}}$

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 $m = -1/2$:

```
-√8 / 15 lower[3 / 2, -1 / 2] / lower[3 / 2, 1 / 2]
-√8 / 15 lower[1, 1] / lower[3 / 2, 1 / 2]

√1 / 15 lower[3 / 2, 1 / 2] / lower[3 / 2, 1 / 2]
√1 / 15 lower[1, 0] / lower[3 / 2, 1 / 2]

√2 / 5 lower[3 / 2, 3 / 2] / lower[3 / 2, 1 / 2]
```

$$-\sqrt{\frac{2}{5}}$$

$$-\frac{2}{\sqrt{15}}$$

$$\frac{1}{\sqrt{15}}$$

$$\frac{1}{\sqrt{30}}$$

$$\sqrt{\frac{3}{10}}$$

so that

$$C(3/3,1,3/2;-3/2,1,-1/2) = -\sqrt{\frac{2}{5}}$$
$$C(3/3,1,3/2;-1/2,0,-1/2) = -2\sqrt{\frac{1}{15}} + \sqrt{\frac{1}{15}} = -\sqrt{\frac{3}{5}}$$
$$C(3/3,1,3/2;1/2,-1,-1/2) = -\frac{1}{3}\sqrt{\frac{2}{5}} + \frac{4}{3}\sqrt{\frac{2}{5}} = \sqrt{\frac{2}{5}}$$

One might expect this result from symmetry, taking into account the minus sign.

Finally for $m = -3/2$:

```
-√2/5 lower[1, 1] / lower[3/2, -1/2]

-√1/15 lower[3/2, -1/2] / lower[3/2, -1/2]
-√1/15 lower[1, 0] / lower[3/2, -1/2]

√8/15 lower[3/2, 1/2] / lower[3/2, -1/2]
```

$$-\frac{2}{\sqrt{15}}$$

$$-\frac{1}{\sqrt{15}}$$

$$-\frac{\sqrt{\frac{2}{5}}}{3}$$

$$\frac{4\sqrt{\frac{2}{5}}}{3}$$

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

```
Solve[{√3/10 x + √3/5 y + √1/10 z == 0,
  -√8/15 x + √1/15 y + √2/5 z == 0, x^2 + y^2 + z^2 == 1}, {x, y, z}]
```

$$\left\{\left\{z \to -\frac{1}{\sqrt{2}}, x \to -\frac{1}{\sqrt{6}}, y \to \frac{1}{\sqrt{3}}\right\}, \left\{z \to \frac{1}{\sqrt{2}}, x \to \frac{1}{\sqrt{6}}, y \to -\frac{1}{\sqrt{3}}\right\}\right\}$$

to get

$$C(3/3,1,3/2;-1/2,1,1/2) = -\sqrt{\frac{1}{6}}$$
$$C(3/3,1,3/2;1/2,0,1/2) = -\sqrt{\frac{1}{3}}$$
$$C(3/3,1,3/2;3/2,-1,1/2) = \sqrt{\frac{1}{2}}$$

where we have chosen a sign convention.

We can do the same for $m = -1/2$:

```
Solve[{√1 / 10 x + √3 / 5 y + √3 / 10 z == 0,
  -√2 / 5 x - √1 / 15 y + √8 / 15 z == 0, x² + y² + z² == 1}, {x, y, z}]
```

$$\left\{\left\{z \to -\frac{1}{\sqrt{6}},\ x \to -\frac{1}{\sqrt{2}},\ y \to \frac{1}{\sqrt{3}}\right\},\ \left\{z \to \frac{1}{\sqrt{6}},\ x \to \frac{1}{\sqrt{2}},\ y \to -\frac{1}{\sqrt{3}}\right\}\right\}$$

to get

$$C(3/3,1,3/2;-3/2,1,-1/2) = \sqrt{\frac{1}{2}}$$
$$C(3/3,1,3/2;-1/2,0,-1/2) = -\sqrt{\frac{1}{3}}$$
$$C(3/3,1,3/2;1/2,-1,-1/2) = \sqrt{\frac{1}{6}}$$

7.7.61 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

```
SphericalHarmonicY[2, 2, θ, ϕ]
```

$$\frac{1}{4} e^{2 i \phi} \sqrt{\frac{15}{2 \pi}} \text{Sin}[\theta]^2$$

```
(-I ℏ) e^(i ϕ) (I D[%, θ] - Cot[θ] D[%, ϕ])
```

```
0
```

(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

```
lowy[y_] := (-I ℏ) Exp[-I ϕ] (-I D[y, θ] - Cot[θ] D[y, ϕ]);
lowyv[m_] = √((2 + m) (2 - m + 1)) ℏ;
```

and apply it repeatedly to Y_{22}:

```
y21 = lowy[SphericalHarmonicY[2, 2, θ, ϕ]] / lowyv[2]
```

$$-\frac{1}{2} e^{i \phi} \sqrt{\frac{15}{2 \pi}} \text{Cos}[\theta] \text{Sin}[\theta]$$

```
y21 - SphericalHarmonicY[2, 1, θ, ϕ]
```

```
0
```

```
y20 = Simplify[lowy[y21] / lowyv[1]]
```

$$\frac{1}{8}\sqrt{\frac{5}{\pi}}\,(1+3\,\text{Cos}[2\,\theta])$$

```
Simplify[y20 - SphericalHarmonicY[2, 0, θ, ϕ]]
```

0

```
y2m1 = lowy[y20] / lowyv[0]
```

$$\frac{1}{4}\,e^{-i\,\phi}\sqrt{\frac{15}{2\,\pi}}\,\text{Sin}[2\,\theta]$$

```
Simplify[y2m1 - SphericalHarmonicY[2, -1, θ, ϕ]]
```

0

```
y2m2 = Simplify[lowy[y2m1]] / lowyv[-1]
```

$$\frac{1}{4}\,e^{-2\,i\,\phi}\sqrt{\frac{15}{2\,\pi}}\,\text{Sin}[\theta]^2$$

```
Simplify[y2m2 - SphericalHarmonicY[2, -2, θ, ϕ]]
```

0

```
lowy[y2m2]
```

0

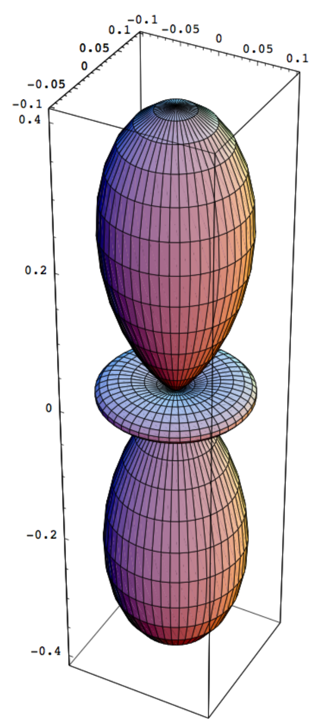
(c) Plot the *shapes* of Y_2^m in 3-dimensions (r, θ, ϕ) using $r = Y_2^m(\theta, \phi)$.

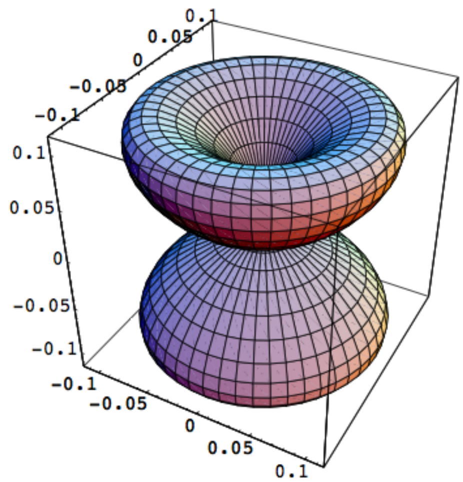
First we create a plotting function

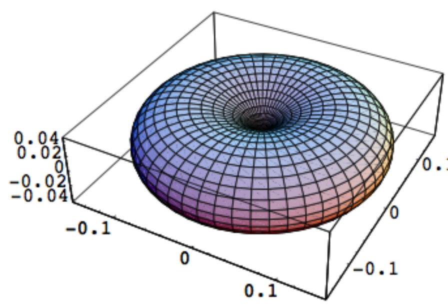
```
ploty[m_] := ParametricPlot3D[
   Conjugate[SphericalHarmonicY[2, m, θ, ϕ]] SphericalHarmonicY[2, m, θ, ϕ]
    {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π}, PlotPoints → 50];
```

and plot $|Y_{2m}|^2$ for $m = 0, 1, 2$:

```
Table[ploty[m], {m, 0, 2}];
```







7.7.62 Starting Point for Shell Model of Nuclei

Consider a three-dimensional isotropic harmonic oscillator with Hamiltonian

$$H = \frac{\vec{p}^2}{2m} + \frac{1}{2} m\omega^2 \vec{r}^2 = \hbar\omega \left(\vec{a}^+ \cdot \vec{a} + \frac{3}{2} \right)$$

where $\vec{p} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$, $\vec{r} = (\hat{x}_1, \hat{x}_2 \hat{x}_2)$, $\vec{a} = (\hat{a}_1, \hat{a}_2, \hat{a}_3)$. We also have the commutators $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$, $[\hat{x}_i, \hat{x}_j] = 0$, $[\hat{p}_i, \hat{p}_j] = 0$, $[\hat{a}_i, \hat{a}_j] = 0$, $[\hat{a}_i^+, \hat{a}_j^+] = 0$, and $[\hat{a}_i, \hat{a}_j^+] = \delta_{ij}$ Answer the following questions.

(a) Clearly, the system is spherically symmetric, and hence there is a conserved angular momentum vector. Show that $\vec{L} = \vec{r} \times \vec{p}$ commutes with the Hamiltonian.

We handle the two terms separately; first the kinetic energy,

$$
\begin{aligned}
\left[L_i, \frac{\vec{p}^2}{2m}\right] &= \epsilon_{ijk}\left[x_j p_k, \frac{p_i p_i}{2m}\right] \\
&= \epsilon_{ijk}\left[x_j p_l p_l\right]\frac{p_k}{2m} = \epsilon_{ijk} 2i\hbar\delta_{jl} p_l \frac{p_k}{2m} \\
&= \frac{i\hbar}{m}\epsilon_{ijk} p_j p_k = 0
\end{aligned}
$$

by the antisymmetry of ϵ_{ijk}. Similarly for the potential energy,

$$
\begin{aligned}
\left[L_i, \frac{1}{2}m\omega^2\vec{x}^2\right] &= \epsilon_{ijk}\left[x_j p_k, \frac{1}{2}m\omega^2 x_l x_l\right] \\
&= \frac{1}{2}m\omega^2\epsilon_{ijk}x_j[p_k, x_l x_l] = -im\hbar\omega^2\epsilon_{ijk}x_j\delta_{kl}x_l \\
&= -im\hbar\omega^2\epsilon_{ijk}x_j x_k = 0
\end{aligned}
$$

by the antisymmetry of ϵ_{ijk}.

(b) Rewrite $\vec{L}$ in terms of creation and annihilation operators.

We generalize the usual creation and annihilation operators for each spatial direction,

$$
a_i = \sqrt{\frac{m\omega}{2\hbar}}\left(x_i + i\frac{p_i}{m\omega}\right) \quad , \quad a_i^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(x_i - i\frac{p_i}{m\omega}\right)
$$

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

$$
x_i = \sqrt{\frac{\hbar}{2m\omega}}(a_i + a_i^+) \quad , \quad p_i = -i\sqrt{\frac{\hbar m\omega}{2}}(a_i - a_i^+)
$$

We find

$$
\begin{aligned}
L_i = \epsilon_{ijk}x_j p_k &= \epsilon_{ijk}\sqrt{\frac{\hbar}{2m\omega}}(a_j + a_j^+)\left(-i\sqrt{\frac{\hbar m\omega}{2}}\right)(a_k - a_k^+) \\
&= -i\frac{\hbar}{2}\epsilon_{ijk}(a_j + a_j^+)(a_k - a_k^+) \\
&= -i\frac{\hbar}{2}\epsilon_{ijk}(a_j a_k - a_j a_k^+ + a_j^+ a_k - a_j^+ a_k^+) \\
&= -i\frac{\hbar}{2}\epsilon_{ijk}(a_j^+ a_k - a_k^+ a_j) \\
&= -i\hbar\epsilon_{ijk}a_j^+ a_k
\end{aligned}
$$

where we have used $\epsilon_{ijk}a_j a_k = \epsilon_{ijk}a_j^+ a_k^+ = 0$, $\epsilon_{ijk}\delta_{kj} = 0$ and $\epsilon_{ijk} = -\epsilon_{ikj}$.

For later purposes, it is useful to define

$$a_+ = -\frac{1}{\sqrt{2}}(a_x - ia_y) \quad , \quad a_- = \frac{1}{\sqrt{2}}(a_x + ia_y)$$

Note that

$$[a_+, a_+^+] = [a_-, a_-^+] = 1$$
$$[a_+, a_-] = [a_+, a_-^+] = [a_+^+, a_-] = [a_+^+, a_-^+] = 0$$

Then the angular momentum operators can be further rewritten as

$$\begin{aligned} L_+ = L_x + iL_y &= -i\hbar(a_y^+ a_z - a_z^+ a_y) + \hbar(a_z^+ a_x - a_x^+ a_z) \\ &= \hbar(-(a_x^+ + ia_y^+)a_z + a_z^+(a_x + ia_y)) \\ &= \hbar\sqrt{2}(a_+^+ a_z + a_z^+ a_-) \end{aligned}$$

$$\begin{aligned} L_- = L_x - iL_y &= -i\hbar(a_y^+ a_z - a_z^+ a_y) - \hbar(a_z^+ a_x - a_x^+ a_z) \\ &= \hbar((a_x^- + ia_y^+)a_z - a_z^+(a_x - ia_y)) \\ &= \hbar\sqrt{2}(a_-^+ a_z + a_z^+ a_+) \end{aligned}$$

$$\begin{aligned} L_z &= -i\hbar(a^+ x a_y - a_y^+ a_x) = -i\hbar\left(\frac{a_-^+ a_+^+}{\sqrt{2}}\frac{a_+ a_+}{\sqrt{2}i} - \frac{a_+^+ a_+^+}{-\sqrt{2}i}\frac{a_- a_+}{\sqrt{2}}\right) \\ &= \hbar(a_+^+ a_+ - a_-^+ a_-) \end{aligned}$$

In other words, $a_+^+(a_+)$ creates (annihilates) the excitation with $L_z = +\hbar$, while $a_-^+(a_-)$ 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

$$\begin{aligned} L_+ |0\rangle &= \hbar\sqrt{2}(a_+^+ a_z + a_z^+ a_-)|0\rangle = 0 \\ L_- |0\rangle &= \hbar\sqrt{2}(a_-^+ a_z + a_z^+ a_+)|0\rangle = 0 \\ L_z |0\rangle &= \hbar(a_+^+ a_+ - a_-^+ a_-)|0\rangle = 0 \end{aligned}$$

(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 $2k+1$ operators T_k^q, $q = k, k-1, ..., -k$ 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,

$$U(R)T_k^q U^+(R) = \sum_{q'} D^{(k)}_{q'\,q} T_k^{q'}$$

To explicitly see the properties of these spherical tensors, it is useful to evaluate the above equation for infinitesimal rotations, for which

$$D^{(k)}_{q'\,q}(\vec{\epsilon}) = \langle k, q'|\, I - i\vec{\epsilon}\cdot\vec{J}/\hbar\, |k, q\rangle = \delta_{q'\,q} - \vec{\epsilon}\cdot\langle k, q'|\, \vec{J}/\hbar\, |k, q\rangle$$

Specifically, consider the infinitesimal rotation $\vec{\epsilon}\cdot\vec{J} = \epsilon J_+$. (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

$$\left(1 - i\epsilon\frac{J_+}{\hbar}\right) T_k^q \left(1 + i\epsilon\frac{J_+}{\hbar}\right) = \sum_q \left(\delta_{q'\,q} - i\epsilon\,\langle k, q'|\, J_+/\hbar\, |k, q\rangle\right) T_k^{q'}$$

and equating terms linear in ϵ we have

$$[J_\pm, T_k^q] = \pm\hbar\sqrt{(k \mp q)(k \pm q + 1)}\,T_k^{q\pm 1}$$
$$[J_z, T_k^q] = \hbar q T_k^q$$

which can be taken as the definitions of spherical tensors. The creation operators are $k = 1$ spherical tensor operators.

$$T^{(1)}_{+1} = a^+_+ \quad , \quad T^{(1)}_0 = a^+_z \quad , \quad T^{(1)}_{-1} = a^+_-$$

To verify this claim:

$$[L_+, T^{(1)}_{+1}] = [\hbar\sqrt{2}(a^+_+ a_z + a^+_z a_-), a^+_+] = 0$$
$$[L_-, T^{(1)}_{+1}] = [\hbar\sqrt{2}(a^+_- a_z + a^+_z a_+), a^+_+] = \hbar\sqrt{2}a^+_z = \hbar\sqrt{2}T^{(1)}_0$$
$$[L_-, T^{(1)}_0] = [\hbar\sqrt{2}(a^+_- a_z + a^+_z a_+), a^+_z] = \hbar\sqrt{2}a^+_- = \hbar\sqrt{2}T^{(1)}_{-1}$$
$$[L_-, T^{(1)}_{-1}] = [\hbar\sqrt{2}(a^+_- a_z + a^+_z a_+), a^+_-] = 0$$

Indeed, the operators form the $k = 1$ representation.

(e) Show that $N = 1$ states, $|1,1,\pm 1\rangle = \mp(a^+_1 \pm a^+_2)\,|0\rangle/\sqrt{2}$ and $|1,1,0\rangle = a^+_3\,|0\rangle$, form the $\ell = 1$ representation. (Notation is $|N, \ell, m\rangle$) It is called a

$1P$ state because it is the first $P-$state.

Using the notation defined above,

$$|1,1,\pm 1\rangle = a_{\pm}^{+}|0\rangle$$

First, we show that $|1,1,1\rangle$ cannot be raised:

$$L_{+}|1,1,1\rangle = \hbar\sqrt{2}(a_{+}^{+}a_z + a_z^{+}a_{-})a_{+}^{+}|0\rangle = 0$$

Then by lowering the state,

$$L_{-}|1,1,1\rangle = \hbar\sqrt{2}(a_{-}^{+}a_z + a_z^{+}a_{+})a_{+}^{+}|0\rangle = \hbar\sqrt{2}a_z^{+}|0\rangle = \hbar\sqrt{2}|1,1,0\rangle$$

Lowering this state once more,

$$L_{-}|1,1,0\rangle = \hbar\sqrt{2}(a_{-}^{+}a_z + a_z^{+}a_{+})a_z^{+}|0\rangle = \hbar\sqrt{2}a_{-}^{+}|0\rangle = \hbar\sqrt{2}|1,1,-1\rangle$$

Finally, this state cannot be lowered

$$L_{-}|1,1,-1\rangle = \hbar\sqrt{2}(a_{-}^{+}a_z + a_z^{+}a_{+})a_{-}^{+}|0\rangle = 0$$

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

$$\begin{aligned}3z^2 - r^2 = 2z^2 - x^2 - y^2 &= \frac{\hbar}{2m\omega}\left(2(a_z + a_z^{+})^2 - (a_x + a_x^{+})^2 - (a_y + a_y^{+})^2\right) \\ &= \frac{\hbar}{2m\omega}\left(2(a_z + a_z^{+})^2 - \frac{1}{2}((a_{-} - a_{+}) + (a_{-}^{+}a_{+}^{+}))^2 - \frac{1}{2}((a_{-} + a_{+}) + (a_{-}^{+} + a_{+}^{+}))^2\right)\end{aligned}$$

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

$$
\begin{aligned}
3z^2 - r^2 \sim & \frac{\hbar}{m\omega}(a_z a_z^+ + a_z^+ a_z) \\
& - \frac{\hbar}{4m\omega}((a_- - a_+)(a_-^+ - a_+^+) + (a_-^+ - a_+^+)(a_- - a_+)) \\
& - \frac{\hbar}{4m\omega}((a_- + a_+)(a_-^+ + a_+^+) + (a_-^+ + a_+^+)(a_- + a_+)) \\
= & \frac{\hbar}{2m\omega}(2(a_z a_z^+ + a_z^+ a_z) - (a_- a_-^+ + a_-^+ a_- + a_+ a_+^+ + a_+^+ a_+)) \\
= & \frac{\hbar}{2m\omega}(2a_z^+ a_z - (a_-^+ a_- + a_+^+ a_+))
\end{aligned}
$$

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,

$$
\begin{aligned}
\langle 1,1,1| \, 3z^2 - r^2 \, |1,1,1\rangle &= \langle 0| \, a_+ \frac{\hbar}{m\omega}(2a_z^+ a_z - (a_-^+ a_- + a_+^+ a_+))a_+^+ \, |0\rangle = -\frac{\hbar}{m\omega} \\
\langle 1,1,0| \, 3z^2 - r^2 \, |1,1,0\rangle &= \langle 0| \, a_z \frac{\hbar}{m\omega}(2a_z^+ a_z - (a_-^+ a_- + a_+^+ a_+))a_z^+ \, |0\rangle = -2\frac{\hbar}{m\omega} \\
\langle 1,1,-1| \, 3z^2 - r^2 \, |1,1,-1\rangle &= \langle 0| \, a_- \frac{\hbar}{m\omega}(2a_z^+ a_z - (a_-^+ a_- + a_+^+ a_+))a_-^+ \, |0\rangle = -\frac{\hbar}{m\omega}
\end{aligned}
$$

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-Gordon coefficients

```
Table[ClebschGordan[{1, m}, {2, 0}, {1, m}], {m, -1, 1}]
```

$$\left\{\frac{1}{\sqrt{10}}, -\sqrt{\frac{2}{5}}, \frac{1}{\sqrt{10}}\right\}$$

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

$$(a_+^+)^2 \, |0\rangle \; , \; (a_z^+)^2 \, |0\rangle \; , \; (a_-^+)^2 \, |0\rangle \; , \; a_+^+ a_z^+ \, |0\rangle \; , \; a_+^+ a_-^+ \, |0\rangle \; , \; a_z^+ a_-^+ \, |0\rangle$$

By looking at the L_z eigenvalues, it is easy to identify

$$\begin{aligned}
|2,2,2\rangle &= \frac{1}{\sqrt{2}}(a_+^\dagger)^2 |0\rangle \\
|2,2,1\rangle &= a_+^\dagger a_z^\dagger |0\rangle \\
|2,2,-1\rangle &= a_z^\dagger a_-^\dagger |0\rangle \\
|2,2,-2\rangle &= \frac{1}{\sqrt{2}}(a_-^\dagger)^2 |0\rangle
\end{aligned}$$

There are two states with $m = 0$: $(a_z^\dagger)^2 |0\rangle$, $a_+^\dagger a_-^\dagger |0\rangle$. We can tell which linear combination belongs to the $l = 2$ representation by acting L_- on $|2,2,1\rangle$,

$$\begin{aligned}
L_- |2,2,1\rangle &= \hbar\sqrt{2}(a_-^\dagger a_z + a_z^\dagger a_+) a_+^\dagger a_z^\dagger |0\rangle \\
&= \hbar\sqrt{2}(a_-^\dagger a_+^\dagger + a_z^\dagger a_z^\dagger) |0\rangle = \hbar\sqrt{6} |2,2,0\rangle
\end{aligned}$$

Therefore we identify

$$|2,2,0\rangle = \frac{1}{\sqrt{3}}(a_-^\dagger a_+^\dagger + a_z^\dagger a_z^\dagger) |0\rangle$$

which is properly normalized as it should be. The orthogonal combination is

$$|2,0,0\rangle = \frac{1}{\sqrt{6}}(2a_-^\dagger a_+^\dagger - a_z^\dagger a_z^\dagger) |0\rangle$$

To verify that this state is indeed an $l = 0$ state, we can check

$$\begin{aligned}
L_+ |2,0,0\rangle &= \hbar\sqrt{2}(a_+^\dagger a_z + a_z^\dagger a_-) \frac{1}{\sqrt{6}}(2a_-^\dagger a_+^\dagger - a_z^\dagger a_z^\dagger) |0\rangle \\
&= \hbar\sqrt{2}\frac{1}{\sqrt{6}}(-a_+^\dagger a_z^\dagger - a_z^\dagger a_+^\dagger + 2a_z^\dagger a_+^\dagger) |0\rangle = 0
\end{aligned}$$

(h) How many possible states are there at the $N = 3, 4$ levels? What ℓ representations do they fall into?

For $N = 3$, it is clear that the state with the highest L_z eigenvalue is $(a_+^\dagger)^3 |0\rangle$ 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 $a_z(a_+^\dagger)^2 |0\rangle$, so there is no orthogonal $l = 2$ representation. However, there are two $m = 1$ states $(a_+^\dagger)^2 a_-^\dagger |0\rangle$ and $(a_z^\dagger)^2 a_-^\dagger |0\rangle$, so there is an orthogonal $l = 1$ representation with 3 states. Finally there are two ways to make an $m = 0$ state, $(a_z^\dagger)^3 |0\rangle$ and $a_z^\dagger a_+^\dagger a_-^\dagger |0\rangle$, 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: $(a_+^+)^2(a_-^+)^2\left|0\right\rangle$, $(a_z^+)^2a_+^+a_-^+\left|0\right\rangle$ and $(a_z^+)^4\left|0\right\rangle$, so there are three total representations. The only $m=3$ state is $a_z^+(a_+^+)^3\left|0\right\rangle$, so there is no $l=3$; there are two $m=2$ states $(a_+^+)^3a_-^+\left|0\right\rangle$ and $a_z^+(a_+^+)^2\left|0\right\rangle$, 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, $N = \textit{even}$ states have even parity, and hence can only have even l, while $N = \textit{odd}$ states have odd parity, and hence odd l. In general, $N = \textit{even}$ states have $l = 0, 2, 4, ..., N$, while $N = \textit{odd}$ 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_z^+, a_+^+, and a_-^+ 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:

$$\begin{aligned}\Pi\,\vec{x}\,\Pi^+ &= e^{i\pi N}\cdot\sqrt{\frac{\hbar}{2m\omega}}(\vec{a}+\vec{a}^+)\cdot e^{-i\pi N} \\ &= \sqrt{\frac{\hbar}{2m\omega}}\sum_m\frac{(i\pi)^m}{m!}[N,[N,[N,.....[N,\vec{a}+\vec{a}^+]......]]]_m\end{aligned}$$

Noting that $[N,a] = -a$ and $[N,a^+] = a^+$, we may collapse this result and separate even and odd terms:

$$\Pi\,\vec{x}\,\Pi^{+} = \sqrt{\frac{\hbar}{2m\omega}} \sum_{m} \frac{(i\pi)^m}{m!} \left((-1)^m \vec{a} + \vec{a}^{+}\right)$$
$$= \sqrt{\frac{\hbar}{2m\omega}} \left((\vec{a} + \vec{a}^{+}) \cos \pi + (-\vec{a} + \vec{a}^{+}) \sin \pi\right) = -\vec{x}$$

$\Pi\,\vec{p}\,\Pi^{+} = -\vec{p}$ follows immediately with

$$\vec{x} \to \vec{p} = -i\sqrt{\frac{\hbar m\omega}{2}}(\vec{a} - \vec{a}^{+})$$

since only the odd term changes sign.

(k) Show that $\Pi = (-1)^N$

The computation is easy:

$$\Pi\,|N,l,m\rangle = e^{i\pi\vec{a}^{+}\cdot\vec{a}}\,|N,l,m\rangle \to \Pi = e^{i\pi N} = (e^{i\pi})^N = (-1)^N$$

(l) Without calculating it explicitly, show that there are no dipole transitions from the $2P$ state to the $1P$ 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 $2P \to 1P$ transition is allowed since $\Delta l = 0$ and $l \neq 0$. However, we note that $2P$ and $1P$ 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.

7.7.63 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.

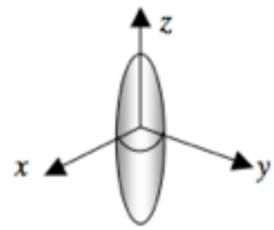


Figure 7.12: Axially Symmetric Rotor

The Hamiltonian for this system is

$$\hat{H} = \frac{\hat{L}_x^2 + \hat{L}_y^2}{2I_\perp} + \frac{\hat{L}_z^2}{2I_\parallel}$$

where $I_\perp$ and $I_\parallel$ are the moments of inertia about the principle axes.

(a) Show that the energy eigenvalues and eigenfunctions are respectively

$$E_{\ell,m} = \frac{\hbar^2}{2I_\perp}\left(\ell(\ell+1) - m^2\left(1 - \frac{I_\perp}{I_\parallel}\right)\right) \quad , \quad \psi_{\ell,m} = Y_\ell^m(\theta,\phi)$$

What are the possible values for ℓ and m? What are the degeneracies?

We seek solutions to $\hat{H}\psi = E\psi$. Note that

$$\hat{L}_x^2 + \hat{L}_y^2 = \hat{L}^2 - \hat{L}_z^2$$

which implies that

$$\hat{H} = \frac{\hat{L}^2}{2I_\perp} - \left(\frac{1}{2I_\perp} - \frac{1}{2I_\parallel}\right)\hat{L}_z^2 = \frac{1}{2I_\perp}\left(\hat{L}^2 - \left(1 - \frac{I_\perp}{I_\parallel}\right)\hat{L}_z^2\right)$$

Now the spherical harmonics are the eigenfunctions of $\hat{L}^2$ and $\hat{L}_z^2$ where

$$\hat{L}^2 Y_\ell^m(\theta,\phi) = \hbar^2\ell(\ell+1)Y_\ell^m(\theta,\phi) \quad , \quad \hat{L}_z Y_\ell^m(\theta,\phi) = \hbar m Y_\ell^m(\theta,\phi)$$

This implies that the energy eigenfunctions are $\psi_{\ell,m} = Y_\ell^m$, i.e.,

$$\hat{H}\psi_{\ell,m} = E_{\ell,m}\psi_{\ell,m}$$
$$E_{\ell,m} = \frac{\hbar^2}{2I_\perp}\left(\ell(\ell+1) - m^2\left(1 - \frac{I_\perp}{I_\parallel}\right)\right)$$

The degeneracy is as follows: if $m \neq 0$, then the two states Y_ℓ^m and Y_ℓ^{-m} have the same energy.

At $t = 0$, the system is prepared in the state

$$\psi_{\ell,m}(t=0) = \sqrt{\frac{3}{4\pi}}\frac{x}{r} = \sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi$$

(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

$$\begin{aligned}
\int d\Omega |\psi_{\ell,m}|^2 &= \int d(\cos\theta)d\phi \frac{3}{4\pi}\sin^2\theta\cos^2\phi \\
&= \int d(\cos\theta)d\phi \frac{3}{4\pi}(1-\cos^2\theta)\cos\theta = \frac{3}{4\pi}\int_{-1}^{1} du(1-u^2)\int_0^{2\pi}\cos^2\phi d\phi \\
&= \frac{3}{4\pi}\left[u - \frac{u^3}{3}\right]_{-1}^{1}\pi = \frac{3}{4\pi}\frac{4}{3}\pi = 1
\end{aligned}$$

(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

$$\begin{aligned}
\frac{1}{\sqrt{2}}\left(-Y_1^1 + Y_1^{-1}\right) &= \frac{1}{\sqrt{2}}\sqrt{\frac{3}{8\pi}}\left(\frac{x+iy}{r} + \frac{x-iy}{r}\right) \\
&= \frac{1}{\sqrt{2}}\sqrt{\frac{3}{8\pi}}\frac{2x}{r} = \sqrt{\frac{3}{4\pi}}\frac{x}{r}
\end{aligned}$$

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_ℓ^2'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 ψ 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 $\ell = 0, 1, 2, ...$ and $m = -\ell, -\ell+1, ...\ell$ for each ℓ 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

$$\ell = 1 \text{ with probability } = 1$$
$$m = +1 \text{ or } m = -1 \text{ with probability } = 1/2 \text{ each}$$

7.7.64 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 $eB > 0$)

$$H = \frac{\Pi_x^2 + \Pi_y^2}{2m} \quad , \quad \Pi_i = p_i - \frac{e}{c}A_i$$

(a) Use the so-called *symmetric gauge* $\vec{A} = B(-y, x)/2$, and simplify the Hamiltonian using two annihilation operators $\hat{a}_x$ and $\hat{a}_y$ for a suitable choice of ω.

We expand the Hamiltonian in the symmetric gauge

$$H = \frac{1}{2m}(\Pi_x^2 + \Pi_y^2) = \frac{1}{2m}\left(\left(p_x - \frac{e}{c}A_x\right)^2 + \left(p_y - \frac{e}{c}A_y\right)^2\right)$$
$$= \frac{1}{2m}\left(\left(p_x + \frac{e}{c}\frac{B}{2}y\right)^2 + \left(p_y - \frac{e}{c}\frac{B}{2}x\right)^2\right)$$

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{e^2B^2}{8mc^2}(x^2 + y^2) + \frac{eB}{2mc}(yp_x - xp_y)$$
$$= \frac{1}{2m}(p_x^2 + p_y^2) + \frac{m\omega^2}{2}(x^2 + y^2) + \omega(yp_x - xp_y)$$

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,

$$\begin{aligned}
H = &-\frac{\hbar\omega}{4}((a_x^+)^2 - a_x^+ a_x - a_x a_x^+ + a_x^2 + (a_y^+)^2 - a_y^+ a_y - a_y a_y^+ + a_y^2) \\
&+ \frac{\hbar\omega}{4}((a_x^+)^2 + a_x^+ a_x + a_x a_x^+ + a_x^2 + (a_y^+)^2 + a_y^+ a_y + a_y a_y^+ + a_y^2) \\
&+ i\frac{\hbar\omega}{2}(a_y^+ a_x^+ - a_y^+ a_x + a_y a_x^+ - a_y a_x - a_x^+ a_y^+ + a_x^+ a_y - a_x a_y^+ + a_x a_y) \\
= &\frac{\hbar\omega}{2}(a_x^+ a_x + a_x a_x^+ + a_y^+ a_y + a_y a_y^+ + 2i(a^+ x a_y - a_y^+ a_x))
\end{aligned}$$

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 $\hat{a}_{\bar{z}} = (\hat{a}_x - i\hat{a}_y)/2$ and then rewrite the Hamiltonian using them. General states are given in the form

$$|n, m\rangle = \frac{(\hat{a}_z^+)^n}{\sqrt{n!}} \frac{(\hat{a}_{\bar{z}}^+)^m}{\sqrt{m!}} |0, 0\rangle$$

starting from the ground state where $\hat{a}_z |0, 0\rangle = \hat{a}_{\bar{z}} |0, 0\rangle = 0$. Show that they are Hamiltonian eigenstates of energies $\hbar\omega(2n + 1)$.

We have

$$a_x = \frac{1}{\sqrt{2}}(a_z + a_{\bar{z}}) \quad , \quad a_y = \frac{1}{\sqrt{2}i}(a_z - a_{\bar{z}})$$

which gives

$$\begin{aligned}
H = &\frac{\hbar\omega}{2}(a_z^+ + a_{\bar{z}}^+)(a_z + a_{\bar{z}}) - \frac{\hbar\omega}{2i}(a_z^+ - a_{\bar{z}}^+)(a_z^+ + a_{\bar{z}}^+) \\
&+ \hbar\omega + \hbar\omega(a_z^+ + a_{\bar{z}}^+)(a_z - a_{\bar{z}}) - \hbar\omega(a_z^- - a_{\bar{z}}^+)(a_z^+ + a_{\bar{z}}^+) \\
= &\hbar\omega(a_z^+ a_z + a_{\bar{z}}^+ a_{\bar{z}}) + \hbar\omega + \frac{\hbar\omega}{2}(a_z^+ a_{\bar{z}} - a_{\bar{z}}^+ a_z + a_{\bar{z}}^+ a_{\bar{z}}) \\
&+ \frac{\hbar\omega}{2}(a_z^+ a_z + a_z^+ a_{\bar{z}} - a_{\bar{z}}^+ a_z - a_{\bar{z}}^+ a_{\bar{z}}) \\
= &\hbar\omega(2a_z^+ a_z + 1)
\end{aligned}$$

Now applying this Hamiltonian to the presumed eigenstates, we have

$$H|n,m\rangle = \hbar\omega(2a_z^+ a_z + 1)\frac{(\hat{a}_z^+)^n}{\sqrt{n!}}\frac{(\hat{a}_{\bar{z}}^+)^m}{\sqrt{m!}}|0,0\rangle$$

We need to commute the a_z through the daggered operators to the right. Let us evaluate the commutation relations:

$$[a_z, a_z^+] = \frac{1}{2}[a_x + ia_y, a_x^+ - ia_y^+] = \frac{1}{2}(1+1) = 1$$
$$[a_z, a_{\bar{z}}^+] = \frac{1}{2}[a_x + ia_y, a_x^+ + ia_y^+] = \frac{1}{2}(1-1) = 0$$

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 $B = 100\,kG$?

For an electron, the Bohr magneton is

$$\mu_B = \frac{e\hbar}{2m_e} = 5.79\times 10^{-11} MeV\,T^{-1}$$

The excitation energy

$$\Delta E = \frac{e\hbar B}{2m_e} = 1.16\times 10^{-3} eV$$

for $B = 100\,kG = 10\,T$. The corresponding thermal energy is

$$\frac{\Delta E}{k} = \frac{1.16\times 10^{-3} eV}{8.62\times 10^{-5} eV\,K^{-1}} = 13.4\,K$$

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

$$\begin{aligned}
a_z|0,0\rangle &= \frac{1}{\sqrt{2}}(a_x + ia_y)|0,0\rangle \\
&= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{i}{m\omega}p_x\right) + i\sqrt{\frac{m\omega}{2\hbar}}\left(y + \frac{i}{m\omega}p_y\right)\right)|0,0\rangle \\
&= \sqrt{\frac{m\omega}{4\hbar}}\left(x + iy + \frac{1}{m\omega}(ip_x - p_y)\right)|0,0\rangle = 0
\end{aligned}$$

which in the position representation is

$$\sqrt{\frac{m\omega}{4\hbar}}\left(x+iy+\frac{1}{m\omega}(i(-i\hbar\partial_x-(-i\hbar\partial_y))\right)\psi_{0,0}$$
$$=\sqrt{\frac{m\omega}{4\hbar}}\left(x+iy+\frac{\hbar}{m\omega}(\partial_x+i\partial_y\right)\psi_{0,0}=0$$

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

$$\sqrt{\frac{m\omega}{4\hbar}}\left(z+\frac{2\hbar}{m\omega}\bar{\partial}\right)\psi_{0,0}=0$$

$$\sqrt{\frac{m\omega}{4\hbar}}\left(\bar{z}+\frac{2\hbar}{m\omega}\partial\right)\psi_{0,0}=0$$

which have the solution

$$\psi_{0,0}\propto e^{-m\omega z\bar{z}/2\hbar}=e^{-m\omega(x^2+y^2)/2\hbar}$$

(e) $|0,m\rangle$ are all ground states. Show that their position-space wave functions are given by

$$\psi_{0,m}(z,\bar{z})=Nz^m e^{-eB\bar{z}z/4\hbar c}$$

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,

$$a_z\psi_{0,m}=\sqrt{\frac{m\omega}{4\hbar}}\left(z+\frac{2\hbar}{m\omega}\bar{\partial}\right)\psi_{0.m}=0$$

and this is clearly met by the form of the given wavefunction. For the second requirement, we use the number operator:

$$a_z^+a_z\,|0,m\rangle=m\,|0,m\rangle$$

In the position representation,

$$\begin{aligned}
a_z^+ &= \frac{1}{\sqrt{2}}(a_x^+ + ia_y^+) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{eB}{4\hbar c}}\left(x - \frac{2c}{eB}ip_x\right) + i\sqrt{\frac{eB}{4\hbar c}}\left(y - \frac{2c}{eB}ip_y\right)\right) \\
&= \sqrt{\frac{eB}{8\hbar c}}\left(x + iy - \frac{2c}{eB}(ip_x - p_y)\right) = \sqrt{\frac{eB}{8\hbar c}}\left(x + iy - \frac{2c}{eB}(i(-i\hbar\partial_x) - i\hbar\partial_y)\right) \\
&= \sqrt{\frac{eB}{8\hbar c}}\left(x + iy - \frac{2\hbar c}{eB}(\partial_x + i\partial_y)\right) = \sqrt{\frac{eB}{8\hbar c}}\left(z - \frac{4\hbar c}{eB}\bar{\partial}\right)
\end{aligned}$$

where ω has been substituted so as not to confuse the eigenvalue m with the mass m. Then, our requirement is

$$\begin{aligned}
&a_z^+ a_z \left|0, m\right\rangle = m\left|0, m\right\rangle \\
&\to \frac{eB}{8\hbar c}\left(z - \frac{4\hbar c}{eB}\bar{\partial}\right)\left(\bar{z} + \frac{4\hbar c}{eB}\partial\right)\psi_{0,m} = m\psi_{0,m} \\
&\to \left(\frac{eB}{8\hbar c}z\bar{z} + \frac{1}{2}z\partial - \frac{1}{2} - \frac{1}{2}\bar{z}\bar{\partial} - 2\frac{\hbar c}{eB}\bar{\partial}\partial\right)\left|0, m\right\rangle = m\left|0, m\right\rangle
\end{aligned}$$

Applying the LHS operator to the given wavefunction, we find

$$\begin{aligned}
&\frac{eB}{8\hbar c}z\bar{z} + \frac{1}{2}z\left(\frac{m}{z} - \frac{eB}{8\hbar c}\bar{z}\right) - \frac{1}{2} - \frac{1}{2}\bar{z}\left(-\frac{eB}{8\hbar c}z\right) - 2\frac{\hbar c}{eB}\bar{\partial}\left(\frac{m}{z} - \frac{eB}{8\hbar c}\bar{z}\right) \\
&= \frac{eB}{8\hbar c}z\bar{z} + \frac{m}{2} - \frac{eB}{8\hbar c}z\bar{z} - \frac{1}{2} + \frac{eB}{8\hbar c}z\bar{z} - 2\frac{\hbar c}{eB}\left(-\frac{eB}{4\hbar c} + \left(\frac{m}{z} - \frac{eB}{4\hbar c}\bar{z}\right)\left(-\frac{eB}{4\hbar c}z\right)\right) \\
&= \frac{m}{2} - \frac{1}{2} + \frac{eB}{8\hbar c}z\bar{z} + \frac{1}{2} + \frac{m}{2} - \frac{eB}{8\hbar c}z\bar{z} \\
&= m
\end{aligned}$$

$\psi_{0,m}$ is indeed the wavefunction $\langle z, \bar{z} \,|\, 0, m\rangle$.

Now let us find N:

$$\begin{aligned}
\int |\psi_{0,m}|^2\, dxdy = N^2 \int dxdy(x^2 + y^2)^m e^{-eN(x^2+y^2)/2\hbar c} \\
= N^2 \int_0^\infty (2\pi r dr) r^{2m} e^{-eBr^2/2\hbar c} = 1 \\
\to N = \left(\int_0^\infty (2\pi r dr) r^{2m} e^{-eBr^2/2\hbar c}\right)^{-1/2}
\end{aligned}$$

Computing

```
(Integrate[2 π r * r^(2 m) * Exp[- (e B)/(2 ℏ c) r^2],
  {r, 0, ∞}, Assumptions → {m > 0, e > 0, B > 0, ℏ > 0, c > 0}])^(-1/2)
```

$$\frac{1}{\sqrt{\pi}\sqrt{2^{1+m}\left(\frac{\hbar c}{B e}\right)^{1+m}\text{Gamma}[1+m]}}$$

We find

$$N = \left(\pi m! \left(\frac{2\hbar c}{eB}\right)^{m+1}\right)^{-1/2}$$

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,

$$\psi_{0,0} \propto e^{-m\omega z\bar{z}/2\hbar} = e^{-m\omega(x^2+y^2)/2\hbar}$$

The correct normalization is easily obtained by the Gaussian integral and we find

$$\psi_{0,0} = \sqrt{\frac{eB}{2\pi\hbar c}}e^{-eBz\bar{z}/4\hbar c}$$

The creation operator was worked out above,

$$a_{z}^{+} = \sqrt{\frac{eB}{8\hbar c}}\left(z - \frac{4\hbar c}{eB}\bar{\partial}\right)$$

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, $\bar{\partial} = -eBz/4\hbar c$ as long as it acts only on the ground state wave functions. therefore,

$$a_{z}^{+} = \sqrt{\frac{eB}{8\hbar c}}\left(z - \frac{4\hbar c}{eB}\frac{-eBz}{4\hbar c}\right) = \sqrt{\frac{eB}{2\hbar c}}z$$

Using the definition,

$$\begin{aligned}\psi_{0,m} &= \frac{(a_{\bar{z}}^{+})^{m}}{\sqrt{m!}}\psi_{0,0} = \frac{1}{\sqrt{m!}}\left(\frac{eB}{2\hbar c}\right)^{m/2} z^{m}\sqrt{\frac{eB}{2\pi\hbar c}}e^{-eBz\bar{z}/4\hbar c} \\ &= \left(\frac{1}{m!}\frac{1}{\pi}\left(\frac{eB}{2\hbar c}\right)^{m+1}\right)^{1/2} z^{m}e^{-eBz\bar{z}/4\hbar c}\end{aligned}$$

which is exactly the same result.

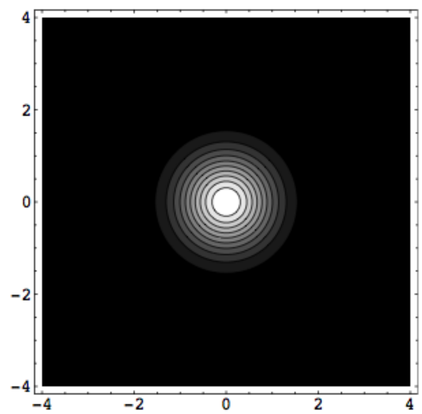
(f) Plot the probability density of the wave function for $m = 0, 3, 10$ on the same scale (use ContourPlot or Plot3D in Mathematica).

Take $eB/2\hbar c = 1$. Then

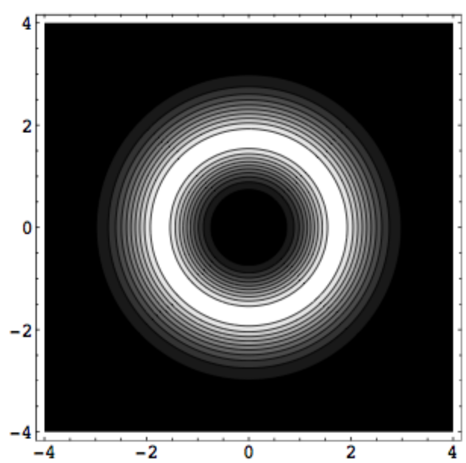
$$\psi_{0,m} = (m!\pi)^{-1/2} z^m e^{-z\bar{z}/2}$$

Therefore,

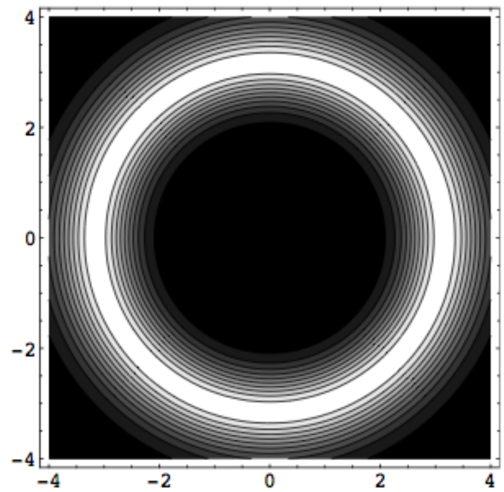
```
ContourPlot[(m ! π)^-1 r^(2 m) E^(-r^2) /. {r -> √(x² + y²)} /. {m → 0},
  {x, -4, 4}, {y, -4, 4}, PlotPoints → 100, PlotRange → {0, 1/π}];
```



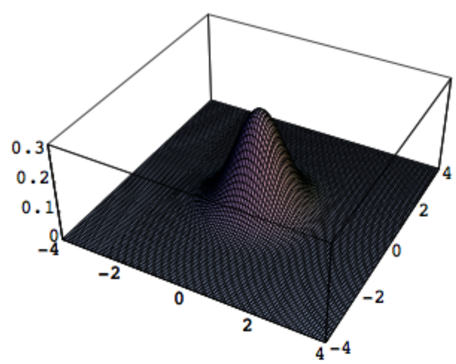

```
ContourPlot[(m ! π)^-1 r^(2 m) E^(-r^2) /. {r -> √(x² + y²)} /. {m → 3},
  {x, -4, 4}, {y, -4, 4}, PlotPoints → 100];
```



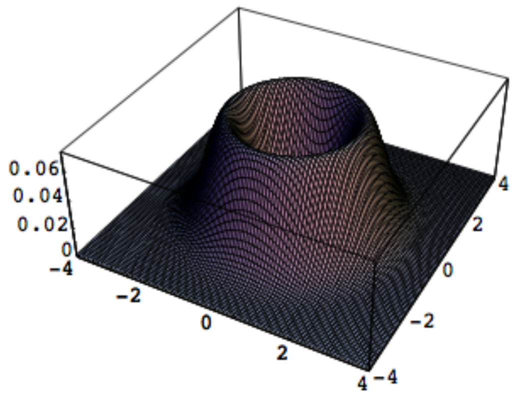
```
ContourPlot[(m! π)^-1 r^(2 m) E^(-r^2) /. {r -> Sqrt[x^2 + y^2]} /. {m → 10},
  {x, -4, 4}, {y, -4, 4}, PlotPoints → 100];
```



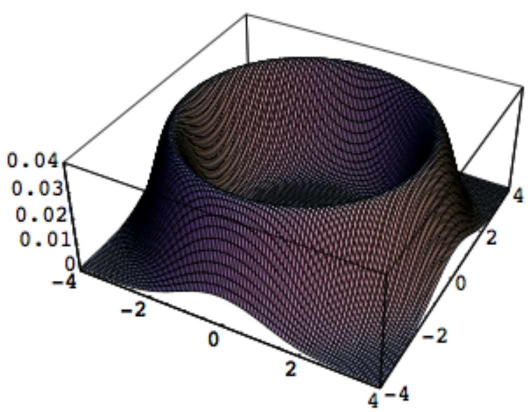

```
Plot3D[(m! π)^-1 r^(2 m) E^(-r^2) /. {r -> Sqrt[x^2 + y^2]} /. {m → 0},
  {x, -4, 4}, {y, -4, 4}, PlotPoints → 100, PlotRange → {0, 1/π}];
```



```
Plot3D[(m! π)^-1 r^(2 m) E^(-r^2) /. {r -> √(x² + y²)} /. {m → 3},
  {x, -4, 4}, {y, -4, 4}, PlotPoints → 100];
```




```
Plot3D[(m! π)^-1 r^(2 m) E^(-r^2) /. {r -> √(x² + y²)} /. {m → 10},
  {x, -4, 4}, {y, -4, 4}, PlotPoints → 100];
```



(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.

```
Solve[D[ (r^n E^(-e B r^2/(4 ℏ)) )^2 , r] == 0, r]
```

$$\left\{\left\{r \to -\frac{\sqrt{2}\sqrt{n}\sqrt{\hbar}}{\sqrt{B}\sqrt{e}}\right\}, \left\{r \to \frac{\sqrt{2}\sqrt{n}\sqrt{\hbar}}{\sqrt{B}\sqrt{e}}\right\}\right\}$$

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 $e^{f\hat{a}_z^+}|0,0\rangle$ represents a near-classical cyclotron motion in position space.

Expanding the state in the Schrodinger picture,

$$\begin{aligned}|\psi_c;t\rangle &= e^{-iHt/\hbar}|\psi_c\rangle = e^{-iHt/\hbar}e^{f\hat{a}_z^+}|0,0\rangle \\ &= \left(\sum \frac{e^{-iHt/\hbar}(fa_z^+)^l}{l!}\right)|0,0\rangle = \left(\sum \frac{e^{-i\omega t(2l+1)}(fa_z^+)^l}{l!}\right)|0,0\rangle \\ &= e^{-i\omega t}\left(\sum (e^{-i2\omega t})^l\frac{(fa_z^+)^l}{l!}\right)|0,0\rangle = e^{-i\omega t}e^{fe^{-i2\omega t}a_z^+}|0,0\rangle\end{aligned}$$

In the position representation

$$a_z^+ = \sqrt{\frac{m\omega}{4\hbar}}\left(\bar{z} - \frac{2\hbar}{m\omega}\partial\right) \equiv \frac{1}{2}k_0\left(\bar{z} - \frac{1}{k_0^2}\partial\right)$$

$$\langle z, \bar{z}\ 0,0\rangle = \frac{1}{\sqrt{\frac{\pi\hbar}{m\omega}}}e^{-m\omega z\bar{z}/2\hbar} \to \sqrt{\frac{2k_0^2}{\pi}}e^{-k_0^2 z\bar{z}}$$

so the wavefunction is

$$\begin{aligned}&\langle z, \bar{z}\,|\,\psi_c;t\rangle \propto e^{-i\omega t}e^{k_0 f e^{-i2\omega t}(\bar{z}-(1/k_0^2)\partial k_0/2}e^{-k_0^2 z\bar{z}} \\ &\to e^{-i\omega t}e^{k_0 f e^{-i2\omega t}\bar{z}}e^{-k_0^2 z\bar{z}}\end{aligned}$$

Making the coordinate transformation $\bar{z} \to \xi/fk_0$,

$$\langle \xi, \bar{\xi}psi_c;t\rangle \propto e^{-i\omega t}e^{\xi e^{-i2\omega t}}e^{-|\xi|^2/|f|^2}$$

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 commnad 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):

```
Table[ContourPlot[Exp[x Cos[2 t] - y Sin[2 t]] Exp[(-x² - y²) / 4],
  {x, -4, 4}, {y, -4, 4}, PlotPoints → 64], {t, 0, 2 π, π / 10}];
```

7.7.65 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 $L = mR^2\dot{\theta}^2/2$ and write down the canonical momentum p_θ 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

$$\dot{x} = -R\dot{\theta}\sin\theta \quad , \quad \dot{y} = R\dot{\theta}\cos\theta$$

and hence

$$L = \frac{1}{2}mR^2\dot{\theta}^2$$

The canonical momentum is given by its definition,

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mR^2\dot{\theta}$$

The Hamiltonian is

$$H = p_\theta\dot{\theta} - L = p_\theta\frac{p_\theta^2}{mR^2} - \frac{1}{2}mR^2\left(\frac{p_\theta^2}{mR^2}\right)^2 = \frac{p_\theta^2}{2mR^2}$$

(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 $\hat{p}_\theta \left| k \right\rangle = \hbar k \left| k \right\rangle$ and show that only $k = n \in \mathbb{Z}$ are allowed because of the requirement $\psi(\theta + 2\pi) = \psi(\theta)$.

The position-space wave function is given by

$$\langle \theta | \, p_\theta \, | k \rangle = \frac{\hbar}{i}\frac{\partial}{\partial\theta} \langle \theta \mid k \rangle = \hbar k \langle \theta \mid k \rangle$$

so that

$$\psi(\theta) = \langle \theta \mid k \rangle = N e^{ik\theta}$$

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 $k =$ 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

$$L_{int} = q\vec{A} \cdot \vec{v} = q(A_x \dot{x} + A_y \dot{y}) = q\frac{Bd^2}{2R^2}(yR\dot{\theta}\sin\theta + xR\dot{\theta}\cos\theta) = \frac{1}{2}qBd^2\dot{\theta}$$

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)

$$\begin{aligned} H &= p_\theta\dot{\theta} - L \\ &= \frac{1}{mR^2}\left(p_\theta - \frac{1}{2}qBd^2\right)^2 \end{aligned}$$

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

$$\frac{q\Phi}{2\hbar} = \frac{qB\pi d^2}{2\pi\hbar} \text{ modulo integers}$$

7.7.66 Density Operators Redux

(a) Find a valid density operator ρ for a spin$-1/2$ system such that

$$\langle S_x \rangle = \langle S_y \rangle = \langle S_z \rangle = 0$$

Remember that for a state represented by a density operator ρ we have $\langle O_q \rangle = Tr[\rho O_q]$. Your density operator should be a 2×2 matrix with trace equal to one and eigenvalues $0 \leq \lambda \leq 1$. Prove that ρ you find does not correspond to a pure state and therefore cannot be represented by a state vector.

We have

$$S_x \leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad S_y \leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad S_z \leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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 ρ 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 ρ 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:

$$\begin{aligned}
|\Psi_i\rangle \leftrightarrow |\Psi_i\rangle \langle\Psi_i| \\
&= \frac{P_i |\Psi\rangle}{\sqrt{\langle\Psi| P_i |\Psi\rangle}} \frac{\langle\Psi| P_i}{\sqrt{\langle\Psi| P_i |\Psi\rangle}} \\
&= \frac{P_i |\Psi\rangle \langle\Psi| P_i}{\langle\Psi| P_i |\Psi\rangle} \\
&= \frac{P_i \rho P_i}{\langle\Psi| P_i |\Psi\rangle}
\end{aligned}$$

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:

$$\begin{aligned}
Tr[\rho P_i] &= [\rho^2 P_i] = Tr[\rho P_i \rho] \\
&= Tr[|\Psi\rangle \langle\Psi| P_i |\Psi\rangle \langle\Psi|] \\
&= \langle\Psi| P_i |\Psi\rangle Tr[|\Psi\rangle \langle\Psi|] \\
&= \langle\Psi| P_i |\Psi\rangle Tr[\rho] = \langle\Psi| P_i |\Psi\rangle
\end{aligned}$$

One could also compute the trace in terms of a complete basis $\{|k\rangle\}$:

$$\begin{aligned}
Tr[\rho P_i] &= \sum_k \langle k| \rho P_i |k\rangle = \sum_k \langle k \mid \Psi\rangle \langle\Psi| P_i |k\rangle \\
&= \sum_k \langle\Psi| P_i |k\rangle \langle k \mid \Psi\rangle = \langle\Psi| P_i \left(\sum_k |k\rangle \langle k|\right) |\Psi\rangle \\
&= \langle\Psi| P_i |\Psi\rangle
\end{aligned}$$

7.7.67 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 $\vec{L} = \vec{r} \times \vec{p}$, so

$$L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

and similarly for the other components, cyclically permuting x, y, z. The first commutator is just hard work:

$$\begin{aligned} L_x L_y &= -\hbar^2 \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right) \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right) \\ &= -\hbar^2 \left(y\frac{\partial}{\partial x} + yz\frac{\partial^2}{\partial z \partial x} - yx\frac{\partial^2}{\partial z^2} - z^2\frac{\partial^2}{\partial y \partial x} + zx\frac{\partial^2}{\partial y \partial z} \right) \end{aligned}$$

Similarly,

$$\begin{aligned} L_y L_x &= -\hbar^2 \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right) \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right) \\ &= -\hbar^2 \left(x\frac{\partial}{\partial y} + zy\frac{\partial^2}{\partial x \partial z} - z^2\frac{\partial^2}{\partial x \partial y} - xy\frac{\partial^2}{\partial z^2} + xz\frac{\partial^2}{\partial z \partial y} \right) \end{aligned}$$

Therefore, since mixed partials are independent of order, we have

$$[L_x, L_y] - i\hbar L_z$$

(b) Show that the operators $L_\pm = L_x \pm i L_y$ 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:

$$[L_\pm, L_z] \mp \hbar L_\pm$$

Thus we have

$$L_z L_\pm |\ell, m\rangle = (L_\pm L_z \pm \hbar L_z) |\ell, m\rangle$$

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 ψ, which is an eigenstate of the operators L^2 and L_z with quantum numbers ℓ and m. Calculate the expectation values $\langle L_x \rangle$ and $\langle L_x^2 \rangle$. HINT: express L_x in terms of $L_\pm$.

We have

$$L_x = \frac{L_+ + L_-}{2}$$

If ψ 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 ℓ, 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 $\hbar^4 m^2/4$ 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 $m = \ell$).

7.7.68 Wave Function Normalizability

The time-independent Schrodinger equation for a spherically symmetric potential $V(r)$ is

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-\frac{\ell(\ell+1)}{r^2}\right]=(E-V)R$$

where $\psi = R(r)Y_\ell^m(\theta,\phi)$, so that the particle is in an eigenstate of angular momentum.

Suppose $R(r) \propto r^{-\alpha}$ and $V(r) \propto -r^{-\beta}$ near the origin. Show that $\alpha < 3/2$ is required if the wavefunction is to be normalizable, but that $\alpha < 1/2$ (or $\alpha < (3-\beta)/2$ if $\beta > 2$) is required for the expectation value of energy to be finite.

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,

$$H\psi = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}(r^2\psi')' - \frac{\ell(\ell+1)}{r^2}\psi\right) + V\psi$$

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 ψ 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.

7.7.69 Currents

The quantum flux density of probability is

$$\vec{j} = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)$$

It is related to the probability density $\rho = |\psi|^2$ by $\nabla \cdot \vec{j} + \dot{\rho} = 0$.

(a) Consider the case where ψ is a stationary state. Show thet ρ and $\vec{j}$ are then independent of time. Show that, in one spatial dimension, $\vec{j}$ is also independent of position.

If ψ is a stationary state, then

$$\psi(t) = \psi(0)e^{-iEt/\hbar}$$

Therefore,

$$\rho(t) = |\psi(t)|^2 = |\psi(0)|^2 = \rho(0) \rightarrow \text{ time-independent}$$

We also have

$$\begin{aligned}\vec{j} &= \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)\\ &= \frac{i\hbar}{2m}(\psi(0)\nabla\psi^*(0) - \psi^*(0)\nabla\psi(0)) \rightarrow \text{ time-independent}\end{aligned}$$

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,

$$\vec{j} = \frac{i\hbar}{2m}(-i\vec{k}|\psi|^2 - i\vec{k}|\psi|^2) = \frac{\hbar\vec{k}}{m}|\psi|^2 = \frac{\hbar\vec{k}}{m}\rho = \rho\vec{v} \rightarrow \text{ the flux density of probability}$$

7.7.70 Pauli Matrices and the Bloch Vector

(a) Show that the Pauli operators

$$\sigma_x = \frac{2}{\hbar}S_x \quad , \quad \sigma_y = \frac{2}{\hbar}S_y \quad , \quad \sigma_z = \frac{2}{\hbar}S_z$$

satisfy

$$Tr[\sigma_i, \sigma_j] = 2\delta_{ij}$$

where the indices i and j can take on the values x, y or z. You will probably want to work with matrix representations of the operators.

We have

$$\sigma_x \leftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_y \leftrightarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma_z \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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:

$$\rho = \frac{1}{2}\left(I + \langle \sigma_x \rangle \sigma_x + \langle \sigma_y \rangle \sigma_y + \langle \sigma_z \rangle \sigma_z\right)$$

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

$$\begin{aligned}|\vec{s}|^2 &= \langle S_x\rangle^2 + \langle S_y\rangle^2 + \langle S_z\rangle^2 \\ &= \frac{\hbar^2}{4}(\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2)\end{aligned}$$

we conclude that $|\vec{s}| = 1$ if and only if the density operator represents a pure state.

Chapter 8

Time-Independent Perturbation Theory

8.9 Problems

8.9.1 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

$$\begin{aligned}
\Delta E_n &= \int_{-\infty}^{\infty} dx \varphi *_n (x) \Delta V(x) \varphi_n(x) \\
&= -\frac{V_0}{L} \int_0^L dx \sin \frac{\pi x}{L} \sin^2 \frac{n\pi x}{L} = -\frac{2V_0}{L} \int_0^L dx \sin \frac{\pi x}{L} \left(1 - \cos \frac{2n\pi x}{L}\right) \\
&= -\frac{V_0}{L} \left[-\frac{L}{\pi} \cos \frac{\pi x}{L}\right]_0^L + \frac{V_0}{L} \int_0^L dx \sin \frac{\pi x}{L} \cos \frac{2n\pi x}{L} \\
&= -\frac{2V_0}{\pi} + \frac{V_0}{2L} \left[\int_0^L dx \sin \frac{(2n+1)\pi x}{L} - \int_0^L dx \sin \frac{(2n-1)\pi x}{L}\right] \\
&= -\frac{2V_0}{\pi} + \frac{V_0}{2L} \left[\frac{L}{(2n+1)\pi} \left[\cos \frac{(2n+1)\pi x}{L}\right]_0^L - \frac{L}{(2n-1)\pi} \left[\cos \frac{(2n-1)\pi x}{L}\right]_0^L\right] \\
&= -\frac{2V_0}{\pi} + \frac{V_0}{2L} \left[\frac{L}{(2n+1)\pi} (-2) - \frac{L}{(2n-1)\pi} (-2)\right] \\
&= -\frac{2V_0}{\pi} + \frac{V_0}{2\pi} \left[\frac{1}{(2n+1)} (-2) - \frac{1}{(2n-1)} (-2)\right] = -\frac{V_0}{\pi} \frac{8n^2}{4n^2 - 1}
\end{aligned}$$

All shifts are negative and for large n, they approach

$$\Delta E_n = -\frac{2V_0}{\pi}$$

independent of n.

8.9.2 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 8.1 below.

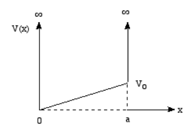


Figure 8.1: Ramp perturbation

We have the perturbation

$$\hat{H}' = \frac{V_0}{a}x \quad , \quad 0 \le x \le a$$

The unperturbed eigenfunctions and corresponding energies (unperturbed) for the first three states are:

$$\begin{aligned} \psi_1^{(0)} &= \sqrt{\tfrac{2}{a}}\sin\tfrac{\pi x}{a} \quad , \quad E_1^{(0)} = \tfrac{\pi^2\hbar^2}{2\mu a^2} \\ \psi_1^{(1)} &= \sqrt{\tfrac{2}{a}}\sin\tfrac{2\pi x}{a} \quad , \quad E_2^{(0)} = \tfrac{2\pi^2\hbar^2}{\mu a^2} \\ \psi_1^{(2)} &= \sqrt{\tfrac{2}{a}}\sin\tfrac{3\pi x}{a} \quad , \quad E_3^{(0)} = \tfrac{9\pi^2\hbar^2}{2\mu a^2} \end{aligned}$$

The 1^{st}−order energy corrections are then

$$\begin{aligned} \left\langle \psi_1^{(0)} \right| \hat{H}' \left| \psi_1^{(0)} \right\rangle &= \tfrac{2}{a}\tfrac{V_0}{a}\int_0^a x\sin^2\tfrac{\pi x}{a}dx = \tfrac{V_0}{2} \\ \left\langle \psi_2^{(0)} \right| \hat{H}' \left| \psi_2^{(0)} \right\rangle &= \tfrac{2}{a}\tfrac{V_0}{a}\int_0^a x\sin^2\tfrac{2\pi x}{a}dx = \tfrac{V_0}{2} \\ \left\langle \psi_3^{(0)} \right| \hat{H}' \left| \psi_3^{(0)} \right\rangle &= \tfrac{2}{a}\tfrac{V_0}{a}\int_0^a x\sin^2\tfrac{3\pi x}{a}dx = \tfrac{V_0}{2} \end{aligned}$$

Therefore, to 1^{st}−order, the perturbed energies are

$$\begin{aligned} E_1 &= \tfrac{\pi^2\hbar^2}{2\mu a^2} + \tfrac{V_0}{2} \\ E_2 &= \tfrac{2\pi^2\hbar^2}{\mu a^2} + \tfrac{V_0}{2} \\ E_3 &= \tfrac{9\pi^2\hbar^2}{2\mu a^2} + \tfrac{V_0}{2} \end{aligned}$$

8.9.3 Weird Perturbation of an Oscillator

A particle of mass m moves in one dimension subject to a harmonic oscillator potential $\frac{1}{2}m\omega^2x^2$. The particle is perturbed by an additional weak anharmonic force described by the potential $\Delta V = \lambda\sin kx$, $\lambda << 1$. Find the corrected ground state.

The zeroth order system is a harmonic oscillator with

$$\begin{aligned}
&\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \\
&\hat{x} = x_0(\hat{a}^+ + \hat{a}) \quad , \quad x_0 = \sqrt{\frac{\hbar}{2m\omega}} \\
&\hat{H}_0 = \hbar\omega\,(\hat{a}^+\hat{a} + 1/2) \rightarrow E_n^{(0)} = \hbar\omega\,(n + 1/2) \\
&\hat{H}_0\,|n\rangle = E_n^{(0)}\,|n\rangle \\
&\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \quad , \quad \hat{a}^+\,|n\rangle = \sqrt{n+1}\,|n+1\rangle
\end{aligned}$$

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

$$\left[\hat{a}, \hat{a}^+\right] = 1$$

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

$$\begin{aligned}
\langle n|\,e^{ikx}\,|0\rangle &= \langle n|\,e^{ik\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^+ + \hat{a})}\,|0\rangle = \langle n|\,e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}^+}e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}}\,|0\rangle\,e^{-\frac{\hbar k^2}{4m\omega}} \\
&= \langle n|\,e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}^+}\sum_{j=0}^{\infty}\frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}\right)^j}{j!}\,|0\rangle\,e^{-\frac{\hbar k^2}{4m\omega}} = \langle n|\,e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}^+}\,|0\rangle\,e^{-\frac{\hbar k^2}{4m\omega}} \\
&= \langle n|\sum_{j=0}^{\infty}\frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}^+\right)^j}{j!}\,|0\rangle\,e^{-\frac{\hbar k^2}{4m\omega}} = \langle n|\sum_{j=0}^{\infty}\frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^j}{j!}\sqrt{j!}\,|j\rangle\,e^{-\frac{\hbar k^2}{4m\omega}} \\
&= \sum_{j=0}^{\infty}\frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^j}{j!}\sqrt{j!}\,\langle n\mid j\rangle\,e^{-\frac{\hbar k^2}{4m\omega}} = \sum_{j=0}^{\infty}\frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^j}{\sqrt{j!}}\delta_{nj}e^{-\frac{\hbar k^2}{4m\omega}} \\
&= \frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^n}{\sqrt{n!}}e^{-\frac{\hbar k^2}{4m\omega}}
\end{aligned}$$

Therefore,

$$\langle n|\sin kx\,|0\rangle = \frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^n}{\sqrt{n!}}e^{-\frac{\hbar k^2}{4m\omega}}\,(1 - (-1)^n)$$

and

$$|0'\rangle = |0\rangle - \frac{\lambda}{\hbar\omega}\sum_{n=odd}\frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^n}{in\sqrt{n!}}e^{-\frac{\hbar k^2}{4m\omega}}|n\rangle$$

$$= |0\rangle - \frac{\lambda}{\hbar\omega}\sum_{q=0}^{\infty}\frac{(-1)^{2q+1}\left(k\sqrt{\frac{\hbar}{2m\omega}}\right)^{2q=1}}{(2q+1)\sqrt{(2q+1)!}}e^{-\frac{\hbar k^2}{4m\omega}}|2q+1\rangle$$

8.9.4 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 8.2 below.

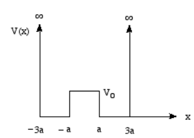


Figure 8.2: Square bump perturbation

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

$$\psi_1^{(0)} = \sqrt{\frac{1}{3a}}\cos\frac{\pi x}{6a} \quad , \quad E_1^{(0)} = \frac{\pi^2\hbar^2}{72ma^2}$$

The 1^{st} order energy correction is

$$E^{(1)} = \left\langle \psi_1^{(0)} \middle| V(x) \middle| \psi_1^{(0)} \right\rangle = \int_{-a}^{a} V_0 \left|\psi_1^{(0)}\right|^2 dx$$

$$= 2V_0\int_0^a \frac{1}{3a}\cos^2\frac{\pi x}{6a}dx = V_0\left(\frac{1}{3}+\frac{\sqrt{3}}{2\pi}\right)$$

Therefore the perturbed energy of the ground state to 1^{st} order is

$$E = E^{(0)} + E^{(1)} = \frac{\pi^2\hbar^2}{72ma^2} + V_0\left(\frac{1}{3}+\frac{\sqrt{3}}{2\pi}\right)$$

8.9.5 Perturbing the 2-dimensional Infinite Square Well

Consider a particle in a 2-dimensional infinite square well given by

$$V(x,y) = \begin{cases} 0 & \text{for } 0 \le x \le a \text{ and } 0 \le y \le a \\ \infty & \text{otherwise} \end{cases}$$

(a) What are the energy eigenvalues and eigenkets for the three lowest levels?

For the unperturbed system we have

$$V(x,y) = \begin{cases} 0 & \text{for } 0 \le x \le a \text{ and } 0 \le y \le a \\ \infty & \text{otherwise} \end{cases}$$

$$\begin{array}{l} \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x) \quad , \quad E_{n_x n_y} = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2\right) \\ \psi_{n_x n_y}(x,y) = \frac{2}{a}\sin\frac{n_x \pi x}{a}\sin\frac{n_y \pi y}{a} \quad , \quad n_x \, , \, n_y = 1, 2, .. \end{array}$$

Ground state:

$$\begin{array}{l} n_x = n_y = 1 \quad , \quad E_{11}^{(0)} = \frac{\pi^2\hbar^2}{ma^2} \\ \psi_{11}^{(0)}(x,y) = \frac{2}{a}\sin\frac{\pi x}{a}\sin\frac{\pi y}{a} \quad , \quad \text{non - degenerate} \end{array}$$

This is a non-degenerate level.

1^{st} **Excited state**:

$$\begin{array}{l} n_x = 1, \, n_y = 2 \quad , \quad E_{12}^{(0)} = \frac{5\pi^2\hbar^2}{2ma^2} \quad , \quad \psi_{12}^{(0)}(x,y) = \frac{2}{a}\sin\frac{\pi x}{a}\sin\frac{2\pi y}{a} \\ n_x = 2, \, n_y = 1 \quad , \quad E_{21}^{(0)} = \frac{5\pi^2\hbar^2}{2ma^2} \quad , \quad \psi_{21}^{(0)}(x,y) = \frac{2}{a}\sin\frac{2\pi x}{a}\sin\frac{\pi y}{a} \end{array}$$

This is a 2-fold degenerate level.

2^{nd} **Excited state**:

$$n_x = n_y = 2 \quad , \quad E_{22}^{(0)} = \frac{4\pi^2\hbar^2}{ma^2} \quad , \quad \psi_{11}^{(0)}(x,y) = \frac{2}{a}\sin\frac{2\pi x}{a}\sin\frac{2\pi y}{a}$$

This is a non-degenerate level.

(b) We now add a perturbation given by

$$V_1(x,y) = \begin{cases} \lambda xy & \text{for } 0 \le x \le a \text{ and } 0 \le y \le a \\ 0 & \text{otherwise} \end{cases}$$

Determine the first order energy shifts for the three lowest levels for $\lambda \ll 1$.

First-order corrections: the perturbation is

$$V_1(x,y) = \begin{cases} \lambda xy & \text{for } 0 \le x \le a \text{ and } 0 \le y \le a \\ 0 & \text{otherwise} \end{cases}$$

Non-degenerate states:

$$\langle 11|\, V_1 \,|11\rangle = \int_0^a\int_0^a \tfrac{4}{a^2}\lambda xy \sin^2\tfrac{\pi x}{a}\sin^2\tfrac{\pi y}{a}dxdy = \tfrac{1}{4}\lambda a^2$$
$$\langle 22|\, V_1 \,|22\rangle = \int_0^a\int_0^a \tfrac{4}{a^2}\lambda xy \sin^2\tfrac{2\pi x}{a}\sin^2\tfrac{2\pi y}{a}dxdy = \tfrac{1}{4}\lambda a^2$$

Therefore, to 1^{st} order:

$$E_{11} = \tfrac{\pi^2\hbar^2}{ma^2} + \tfrac{1}{4}\lambda a^2$$
$$E_{22} = \tfrac{4\pi^2\hbar^2}{ma^2} + \tfrac{1}{4}\lambda a^2$$

Degenerate states: we must diagonalize a 2×2 matrix. We have

$$\langle 12|\, V_1 \,|12\rangle = \int_0^a\int_0^a \tfrac{4}{a^2}\lambda xy \sin^2\tfrac{\pi x}{a}\sin^2\tfrac{2\pi y}{a}dxdy = \tfrac{1}{4}\lambda a^2 = \langle 22|\, V_1 \,|22\rangle$$
$$\langle 12|\, V_1 \,|21\rangle = \int_0^a\int_0^a \tfrac{4}{a^2}\lambda xy \sin\tfrac{2\pi x}{a}\sin\tfrac{\pi y}{a}\sin\tfrac{\pi x}{a}\sin\tfrac{2\pi y}{a}dxdy = \tfrac{256}{81\pi^4}\lambda a^2 = \langle 21|\, V_1 \,|12\rangle$$

Therefore, the degenerate submatirx (to be diagonalized) is

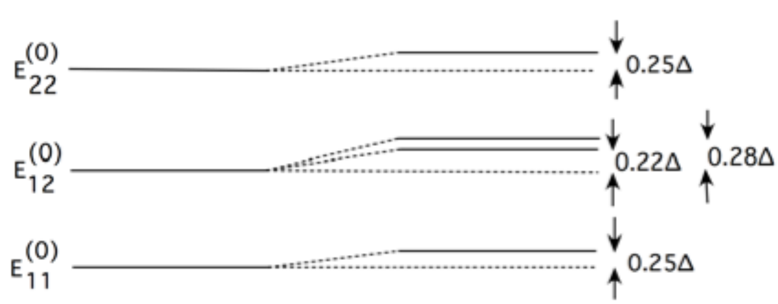
$$\frac{1}{4\pi^4}\lambda a^2 \begin{pmatrix} \pi^4 & \frac{1024}{81} \\ \frac{1024}{81} & \pi^4 \end{pmatrix}$$

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:



8.9.6 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 8.3 below.

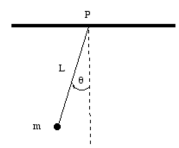


Figure 8.3: A quantum pendulum

(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

$$\psi_0 = \sqrt{\frac{\alpha}{\pi^{1/2}}}e^{-\frac{1}{2}\alpha^2x^2} \quad , \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}$$

Therefore, the lowest order correction to the ground state energy is

$$E_0^{(1)} = -\frac{1}{24}\frac{mg}{\ell^3}\langle 0|\, x^4 \,|0\rangle = -\frac{1}{24}\frac{mg}{\ell^3}\frac{\alpha}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty} x^4 e^{-\alpha^2x^2}dx = -\frac{1}{32}\frac{\hbar^2}{m\ell^2}$$

8.9.7 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

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \quad , \quad \hat{H}'(x) = \alpha\hat{x}^3 + \beta\hat{x}^4$$

with

$$\hat{x} = x_0(\hat{a} + \hat{a}^+) \quad , \quad x_0 = \sqrt{\tfrac{\hbar}{2m\omega}}$$
$$\hat{H}_0 = \hbar\omega\left(\hat{a}^+\hat{a} + 1/2\right) \to E_n^{(0)} = \hbar\omega\left(n + 1/2\right)$$
$$\hat{H}_0\left|n\right\rangle = E_n^{(0)}\left|n\right\rangle$$

and

$$\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle \quad , \quad \hat{a}^+\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle$$

We then have

$$\left\langle n'\right|\hat{x}\left|n\right\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\left\langle n'\right|\hat{a}\left|n\right\rangle + \left\langle n'\right|\hat{a}^+\left|n\right\rangle\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right)$$

From this result we get

$$\begin{aligned}\left\langle n'\right|\hat{x}^2\left|n\right\rangle &= \sum_m \left\langle n'\right|\hat{x}\left|m\right\rangle\left\langle m\right|\hat{x}\left|n\right\rangle \\ &= \frac{\hbar}{2m\omega}\sum_m\left(\sqrt{m}\delta_{n',m-1} + \sqrt{m+1}\delta_{n',m+1}\right)\left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right) \\ &= \frac{\hbar}{2m\omega}\left(\sqrt{n(n-1)}\delta_{n',n-2} + \sqrt{(n+1)(n+2)}\delta_{n',n+2} + (2n+1)\delta_{n',n}\right)\end{aligned}$$

and

$$\begin{aligned}\left\langle n'\right|\hat{x}^3\left|n\right\rangle &= \sum_m \left\langle n'\right|\hat{x}^2\left|m\right\rangle\left\langle m\right|\hat{x}\left|n\right\rangle \\ &= \left(\frac{\hbar}{2m\omega}\right)^{3/2}\sum_m\begin{pmatrix}\sqrt{m(m-1)}\delta_{n',m-2} \\ +\sqrt{(m+1)(m+2)}\delta_{n',m+2} + (2m+1)\delta_{n',m}\end{pmatrix} \\ &\qquad\times\left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right) \\ &= \left(\frac{\hbar}{2m\omega}\right)^{3/2}\begin{pmatrix}\sqrt{n(n-1)(n-2)}\delta_{n',n-3} + 3n\sqrt{n}\delta_{n',n-1} \\ +(3n+2)\sqrt{n+1}\delta_{n',n+1} + \sqrt{(n+1)(n+2)(n+3)}\delta_{n',n+3}\end{pmatrix}\end{aligned}$$

and

$$\langle n'|\hat{x}^4|n\rangle = \sum_m \langle n'|\hat{x}^2|m\rangle\langle m|\hat{x}^2|n\rangle$$

$$= \left(\frac{\hbar}{2m\omega}\right)^2 \sum_m \left(\begin{array}{l}\sqrt{m(m-1)}\delta_{n',m-2} \\ +\sqrt{(m+1)(m+2)}\delta_{n',m+2} + (2m+1)\delta_{n',m}\end{array}\right) \times \left(\begin{array}{l}\sqrt{n(n-1)}\delta_{m,n-2} \\ +\sqrt{(n+1)(n+2)}\delta_{m,n+2} + (2n+1)\delta_{m,n}\end{array}\right)$$

$$= \left(\frac{\hbar}{2m\omega}\right)^2 \left(\begin{array}{l}\sqrt{n(n-1)(n-2)(n-3)}\delta_{n',n-4} + 2(2n-1)\sqrt{n(n-1)}\delta_{n',n-2} \\ +3(2n^2+2n+1)\delta_{n',n} + 4(n+1)\sqrt{(n+1)(n+2)}\delta_{n',n+2} \\ +\sqrt{(n+1)(n+2)(n+3)(n+4)}\delta_{n',n+4}\end{array}\right)$$

Using these matrix elements, we get

$$E_n^{(1)} = \langle n|\hat{H}'|n\rangle = \alpha\langle n|\hat{x}^3|n\rangle + \beta\langle n|\hat{x}^4|n\rangle = \beta\langle n|\hat{x}^4|n\rangle$$
$$= 3(2n^2+2n+1)\beta\left(\frac{\hbar}{2m\omega}\right)^2$$

so that to 1^{st}-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 $1^{st}-$order.

The state vector to $1^{st}-$order is

$$|N\rangle = |n\rangle + \sum_{m\neq n}\frac{\langle m|\hat{H}'|n\rangle}{E_n^{(0)}-E_m^{(0)}}|m\rangle = |n\rangle + \frac{1}{\hbar\omega}\sum_{m\neq n}\frac{\langle m|\hat{H}'|n\rangle}{n-m}|m\rangle$$
$$= |n\rangle + a_{n-4}|n-4\rangle + a_{n-3}|n-3\rangle + a_{n-2}|n-2\rangle + a_{n-1}|n-1\rangle$$
$$+ a_{n+1}|n+1\rangle + a_{n+2}|n+2\rangle + a_{n+3}|n+3\rangle + a_{n+4}|n+4\rangle$$

where

$$a_{n-4} = \beta\left(\tfrac{\hbar}{2m\omega}\right)^2\sqrt{n(n-1)(n-2)(n-3)} \quad , \quad a_{n-3} = \alpha\left(\tfrac{\hbar}{2m\omega}\right)^{3/2}\sqrt{n(n-1)(n-2)}$$
$$a_{n-2} = 2\beta\left(\tfrac{\hbar}{2m\omega}\right)^2(n-1)\sqrt{n(n-1)} \quad , \quad a_{n-1} = 3\alpha\left(\tfrac{\hbar}{2m\omega}\right)^{3/2}n\sqrt{n}$$
$$a_{n+2} = 4\beta\left(\tfrac{\hbar}{2m\omega}\right)^2(n+1)\sqrt{(n+1)(n+2)} \quad , \quad a_{n+1} = \alpha\left(\tfrac{\hbar}{2m\omega}\right)^{3/2}(2+3n)\sqrt{n+1}$$
$$a_{n+4} = \beta\left(\tfrac{\hbar}{2m\omega}\right)^2\sqrt{(n+1)(n+2)(n+3)(n+4)} \quad , \quad a_{n+3} = \alpha\left(\tfrac{\hbar}{2m\omega}\right)^{3/2}\sqrt{(n+1)(n+2)(n+3)}$$

8.9.8 A Relativistic Correction for Harmonic Oscillator

A particle of mass m moves in a $1-$dimensional oscillator potential

$$V(x) = \frac{1}{2}m\omega^2x^2$$

In the nonrelativistic limit, where the kinetic energy and the momentum are related by

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

the ground state energy is well known to be $E_0 = \hbar\omega/2$.

Relativistically, the kinetic energy and the momentum are related by

$$T = E - mc^2 = \sqrt{m^2c^4 + p^2c^2} - mc^2$$

(a) Determine the lowest order correction to the kinetic energy (a p^4 term).

We have

$$\begin{aligned} T = E - mc^2 &= \sqrt{m^2c^4 + p^2c^2} - mc^2 = mc^2\left(\sqrt{1 + \frac{p^2}{m^2c^2}} - 1\right) \\ &\approx mc^2\left(1 + \frac{p^2}{2m^2c^2} - \frac{p^4}{8m^4c^4} + ... - 1\right) = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} \end{aligned}$$

including only the largest correction.

Therefore,

$$\begin{aligned} H = T + V &= \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \frac{1}{2}m\omega^2x^2 \\ &= \left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2\right) - \frac{p^4}{8m^3c^2} \end{aligned}$$

(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

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \rightarrow \text{ a 1 - dimensional harmonic oscillator}$$

where

$$E_n^{(0)} = \hbar\omega(n + 1/2) \quad , \quad \hat{H}_0 \left|n\right\rangle = E_n^{(0)} \left|n\right\rangle$$

and the perturbation is

$$H_1 = -\frac{p^4}{8m^3c^2}$$

The energy correction for the ground state is then

$$E_0^{(1)} = \left\langle 0\right| \hat{H}_1 \left|0\right\rangle = -\frac{1}{8m^3c^2} \left\langle 0\right| \hat{p}^4 \left|0\right\rangle$$

where

$$\hat{p} = ip_0(\hat{a}^+ - \hat{a}) \ , \ p_0 = \sqrt{\frac{\hbar m\omega}{2}}$$

Thus,

$$\begin{aligned}
E_0^{(1)} &= -\frac{\hbar^2\omega^2}{32mc^2} \langle 0| (\hat{a}^+ - \hat{a})^4 |0\rangle \\
&= -\frac{\hbar^2\omega^2}{32mc^2} \langle 0| (\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a}) |0\rangle \\
&= \frac{\hbar^2\omega^2}{32mc^2} \langle 0| \hat{a}(\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a})\hat{a}^+ |0\rangle = \frac{\hbar^2\omega^2}{32mc^2} \langle 1| (\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a}) |1\rangle \\
&= \frac{\hbar^2\omega^2}{32mc^2} \langle 1| (\hat{a}^+ - \hat{a}) \left(\sqrt{2}\,|2\rangle - |0\rangle\right) = \frac{\hbar^2\omega^2}{32mc^2} \langle 1| \left(\sqrt{6}\,|3\rangle - 3\,|1\rangle\right) \\
&= -\frac{3\hbar^2\omega^2}{32mc^2}
\end{aligned}$$

8.9.9 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)

$$\begin{aligned}
&|+1\rangle \to E_{+1}^{(0)} = A\hbar^2 \\
&|0\rangle \to E_0^{(0)} = 0 \\
&|-1\rangle \to E_{-1}^{(0)} = A\hbar^2
\end{aligned}$$

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

$$\hat{V} = B(\hat{S}_x^2 - \hat{S}_y^2) = \frac{1}{4}B\left(\left(\hat{S}_+ + \hat{S}_-\right)^2 + \left(\hat{S}_+ - \hat{S}_-\right)^2\right) = \frac{1}{2}B\left(\left(\hat{S}_+\right)^2 + \left(\hat{S}_-\right)^2\right)$$

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-denegerate

(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 1^{st}-order perturbation theory result. This means that there are no higher order correction in perturbation theory.

8.9.10 Perturbation Theory in Two-Dimensional Hilbert Space

Consider a spin$-1/2$ particle in the presence of a static magnetic field along the z and x directions,

$$\vec{B} = B_z \hat{e}_z + B_x \hat{e}_x$$

(a) Show that the Hamiltonian is

$$\hat{H} = \hbar\omega_0 \hat{\sigma}_z + \frac{\hbar\Omega}{2}\hat{\sigma}_x$$

where $\hbar\omega_0 = \mu_B B_z$ and $\hbar\Omega_0 = 2\mu_B B_x$.

The Hamiltonian is

$$\begin{aligned}\hat{H} &= -\vec{\mu}\cdot\vec{B} = -(-2\frac{\mu_B}{\hbar}\vec{S})\cdot\vec{B} = \mu_B\vec{\sigma}\cdot\vec{B} \\ &= \mu_B\sigma_x B_x + \mu_B\sigma_z B_z = \hbar\omega_0\sigma_z + \frac{\hbar\Omega}{2}\sigma_x\end{aligned}$$

where

$$\hbar\omega_0 = \mu_B B_z \quad , \quad \frac{\hbar\Omega}{2} = \mu_B B_x$$

(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 $|B_x| << |B_z|$ and use perturbation theory with

$$\hat{H}_1 = \frac{\hbar\Omega}{2}\sigma_x$$

The first-order correction vanishes since

$$E_\uparrow^{(1)} = \langle\uparrow|\,\hat{H}_1\,|\uparrow\rangle = \tfrac{\hbar\Omega}{2}\,\langle\uparrow|\,\sigma_x\,|\uparrow\rangle = 0$$
$$E_\downarrow^{(1)} = \langle\downarrow|\,\hat{H}_1\,|\downarrow\rangle = \tfrac{\hbar\Omega}{2}\,\langle\downarrow|\,\sigma_x\,|\downarrow\rangle = 0$$

The second-order shift is

$$E_\uparrow^{(2)} = \frac{\left|\langle\downarrow|\hat{H}_1|\uparrow\rangle\right|^2}{E_\uparrow^{(0)}-E_\downarrow^{(0)}} = \left(\tfrac{\hbar\Omega}{2}\right)^2\frac{|\langle\downarrow|\sigma_x|\uparrow\rangle|^2}{2\hbar\omega_0} = \tfrac{\hbar\omega_0}{2}\left(\tfrac{\Omega}{2\omega_0}\right)^2 = \tfrac{\hbar\omega_0}{2}\left(\tfrac{B_x}{B_z}\right)^2$$
$$E_\downarrow^{(2)} = \frac{\left|\langle\downarrow|\hat{H}_1|\uparrow\rangle\right|^2}{E_\downarrow^{(0)}-E_\uparrow^{(0)}} = \left(\tfrac{\hbar\Omega}{2}\right)^2\frac{|\langle\downarrow|\sigma_x|\uparrow\rangle|^2}{-2\hbar\omega_0} = -\tfrac{\hbar\omega_0}{2}\left(\tfrac{B_x}{B_z}\right)^2$$

Thus, to second-order we have

$$E_\uparrow = \hbar\omega_0 + \tfrac{\hbar\omega_0}{2}\left(\tfrac{B_x}{B_z}\right)^2 = \hbar\omega_0\left(1+\tfrac{1}{2}\left(\tfrac{B_x}{B_z}\right)^2\right)$$
$$E_\downarrow = -\hbar\omega_0 - \tfrac{\hbar\omega_0}{2}\left(\tfrac{B_x}{B_z}\right)^2 = -\hbar\omega_0\left(1+\tfrac{1}{2}\left(\tfrac{B_x}{B_z}\right)^2\right)$$

The lowest order corrections to the state vectors are:

$$|\uparrow_z\rangle \Rightarrow |\uparrow_z\rangle + |\downarrow_z\rangle\,\frac{\langle\downarrow|\hat{H}_1|\uparrow\rangle}{E_\downarrow^{(0)}-E_\uparrow^{(0)}} = |\uparrow_z\rangle + \tfrac{1}{2}\tfrac{B_x}{B_z}\,|\downarrow_z\rangle$$
$$|\downarrow_z\rangle \Rightarrow |\downarrow_z\rangle - |\uparrow_z\rangle\,\frac{\langle\uparrow|\hat{H}_1|\downarrow\rangle}{E_\uparrow^{(0)}-E_\downarrow^{(0)}} = |\downarrow_z\rangle - \tfrac{1}{2}\tfrac{B_x}{B_z}\,|\uparrow_z\rangle$$

(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

$$|\uparrow_x\rangle \Rightarrow E_\uparrow^{(0)} = \tfrac{\hbar\Omega}{2}$$
$$|\downarrow_x\rangle \Rightarrow E_\downarrow^{(0)} = -\tfrac{\hbar\Omega}{2}$$

Now we add a small field $|B_z| << |B_x|$ and use perturbation theory with

$$\hat{H}_1 = \hbar\omega_0\sigma_z$$

The first-order correction vanishes since

$$\begin{aligned} E_\uparrow^{(1)} &= \langle\uparrow|\hat{H}_1|\uparrow\rangle = \hbar\omega_0\langle\uparrow|\sigma_z|\uparrow\rangle = 0 \\ E_\downarrow^{(1)} &= \langle\downarrow|\hat{H}_1|\downarrow\rangle = \hbar\omega_0\langle\downarrow|\sigma_z|\downarrow\rangle = 0 \end{aligned}$$

The second-order shift is

$$\begin{aligned} E_\uparrow^{(2)} &= \frac{\left|\langle\downarrow|\hat{H}_1|\uparrow\rangle\right|^2}{E_\uparrow^{(0)}-E_\downarrow^{(0)}} = (\hbar\omega_0)^2\frac{|\langle\downarrow|\sigma_z|\uparrow\rangle|^2}{\hbar\Omega} = \frac{\hbar\Omega}{4}\left(\frac{2\omega_0}{\Omega}\right)^2 = \frac{\hbar\Omega}{4}\left(\frac{B_z}{B_x}\right)^2 \\ E_\downarrow^{(2)} &= \frac{\left|\langle\downarrow|\hat{H}_1|\uparrow\rangle\right|^2}{E_\downarrow^{(0)}-E_\uparrow^{(0)}} = (\hbar\omega_0)^2\frac{|\langle\downarrow|\sigma_x|\uparrow\rangle|^2}{-\hbar\Omega} = -\frac{\hbar\Omega}{4}\left(\frac{B_z}{B_x}\right)^2 \end{aligned}$$

Thus, to second-order we have

$$\begin{aligned} E_\uparrow &= \frac{\hbar\Omega}{2} + \frac{\hbar\Omega}{4}\left(\frac{B_z}{B_x}\right)^2 = \frac{\hbar\Omega}{2}\left(1+\frac{1}{2}\left(\frac{B_z}{B_x}\right)^2\right) \\ E_\downarrow &= -\frac{\hbar\Omega}{2} - \frac{\hbar\Omega}{4}\left(\frac{B_z}{B_x}\right)^2 = -\frac{\hbar\Omega}{2}\left(1+\frac{1}{2}\left(\frac{B_z}{B_x}\right)^2\right) \end{aligned}$$

(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

$$\begin{aligned} &\det(\hat{H} - \hbar\lambda\hat{I}) = \hbar^2\left[(\omega_0-\lambda)(-\omega_0-\lambda) - \frac{\Omega^2}{4}\right] = 0 \\ &\lambda_\pm = \pm\sqrt{\omega_0^2 + \frac{\Omega^2}{4}} \Rightarrow E_\pm = \pm\hbar\sqrt{\omega_0^2+\frac{\Omega^2}{4}} \end{aligned}$$

The eigenvectors are

$$\begin{aligned} &\hat{H}|\pm\rangle = E_\pm|\pm\rangle \\ &|\pm\rangle = \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} \Rightarrow \omega_0 a_\pm + \frac{\Omega}{2}b_\pm = \lambda_\pm a_\pm \\ &unnormalized: a_\pm = 1 \rightarrow b_\pm = \frac{\lambda_\pm - \omega_0}{\Omega/2} \\ &|\pm\rangle = N_\pm\left[\frac{\Omega}{2}|\uparrow_z\rangle + (\lambda_\pm - \omega_0)|\downarrow_z\rangle\right] \end{aligned}$$

Let us now expand to lowest non-vanishing order in the small parameter

$$\varepsilon = \frac{\Omega}{2\omega_0} = \frac{1}{2}\frac{B_x}{B_z}$$

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

$$\lambda_\pm - \omega_0 = \omega_0(\pm\sqrt{1+\varepsilon^2} + -1) = \begin{cases} \frac{\varepsilon^2}{2}\omega_0 & + \\ -2\omega_0 & - \end{cases}$$

so that

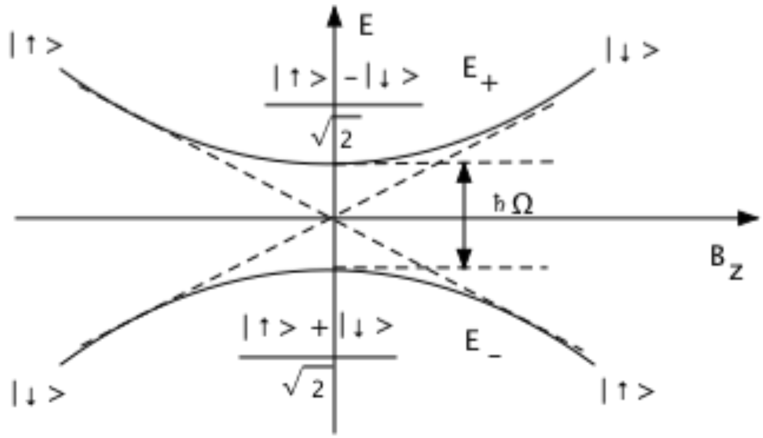
$$|+\rangle = N_+\left[\frac{\Omega}{2}|\uparrow_z\rangle + (\lambda_+ - \omega_0)|\downarrow_z\rangle\right] = N_+\left[\frac{\Omega}{2}|\uparrow_z\rangle + \frac{\varepsilon^2}{2}\omega_0|\downarrow_z\rangle\right]$$
$$= N_+\left[|\uparrow_z\rangle - \frac{\Omega}{4\omega_0}|\downarrow_z\rangle\right]$$

$$|-\rangle = N_-\left[\frac{\Omega}{2}|\uparrow_z\rangle + (\lambda_- - \omega_0)|\downarrow_z\rangle\right] = N_-\left[\frac{\Omega}{2}|\uparrow_z\rangle - 2\omega_0|\downarrow_z\rangle\right]$$
$$= N_-\left[|\downarrow_z\rangle - \frac{\Omega}{4\omega_0}|\uparrow_z\rangle\right]$$

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 $B_z = 0$ (as shown above the dotted lines). Including B_x the degeneracy is broken; the new eigenvectors are symmetric and antisymmetric combinations of $|\uparrow\rangle$ and $|\downarrow\rangle$.

8.9.11 Finite Spatial Extent of the Nucleus

In most discussions of atoms, the nucleus is treated as a positively charged point particle. In fact, the nucleus does possess a finite size with a radius given approximately by the empirical formula

$$R \approx r_0 A^{1/3}$$

where $r_0 = 1.2 \times 10^{-13}\, cm$ (i.e., 1.2 Fermi) and A is the atomic weight or number (essentially the number of protons and neutrons in the nucleus). A reasonable assumption is to take the total nuclear charge $+Ze$ as being uniformly distributed over the entire nuclear volume (assumed to be a sphere).

(a) Derive the following expression for the electrostatic potential energy of an electron in the field of the *finite* nucleus:

$$V(r) = \begin{cases} -\frac{Ze^2}{r} & \text{for } r > R \\ \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2}\right) & \text{for } r < R \end{cases}$$

Draw a graph comparing this potential energy and the point nucleus potential energy.

For $r > R$, Gauss' law says that the sphere of charge acts like a point charge at the center of the sphere. Therefore,

$$V(r) = -\frac{Ze^2}{r} r > R$$

For $r < R$, Gauss's law says that only the charge inside contributes. Therefore,

$$\oint_S \vec{\varepsilon} \cdot d\vec{A} = \varepsilon_r 4\pi r^2 = 4\pi(\text{chargeinside}) = 4\pi Ze\frac{r^3}{R^3}$$
$$\varepsilon_r = Ze\frac{r}{R^3} \to \varphi = Ze\frac{r^2}{2R^3} + C = textpotential$$
$$\to V(r) = Ze^2\frac{r^2}{2R^3} + C = \text{ potential energy}$$

Now, continuity at $r - R$ gives

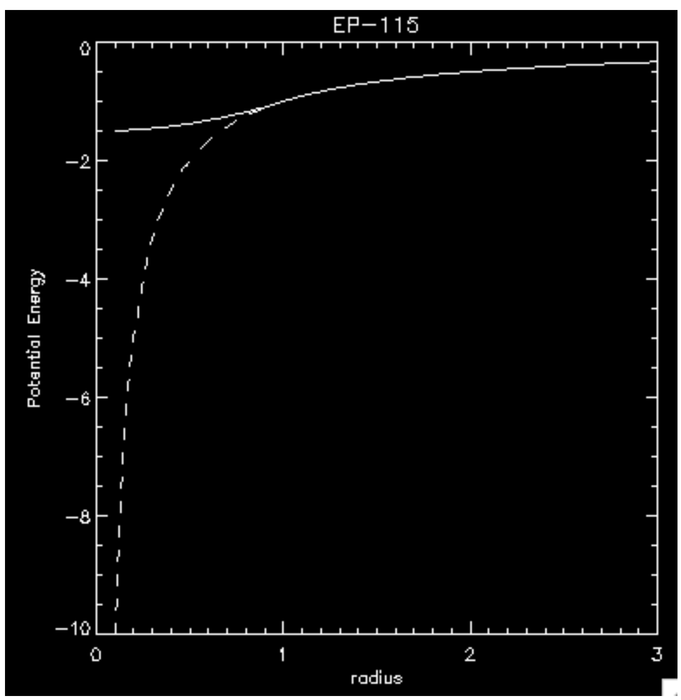
$$Ze^2\frac{R^2}{2R^3} + C = -\frac{Ze^2}{R} \to C = -\frac{3Ze^2}{2R}$$

Therefore,

$$V(r) = \begin{cases} -\frac{Ze^2}{r} & r > R \\ \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2}\right) & r < R \end{cases}$$

The graph below chooses $Ze^2 = 1$ and $R = 1$ or

$$V(r) = \begin{cases} -\frac{1}{r} & r > 1 \\ \frac{r^2}{2} - \frac{3}{2} & r < 1 \end{cases}$$



(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

$$\hat{H} = \frac{\vec{p}^2}{2m} + V(r) = \frac{\vec{p}^2}{2m} - \frac{Ze^2}{r} + \left(V(r) + \frac{Ze^2}{r}\right)$$
$$\hat{H}_0 = \frac{\vec{p}^2}{2m} - \frac{Ze^2}{r} \rightarrow \text{ point charge at origin (hydrogen - like)}$$

$$\hat{H}_1 = V(r) + \frac{Ze^2}{r} = \begin{cases} 0 & r > R \\ \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2}\right) + \frac{Ze^2}{r} & r < R \end{cases}$$

(c) Calculate(remember that $R \ll a_0 =$ Bohr radius) the $1^{st}-$order perturbed energy for the $1s$ $(n\ell m) = (100)$ state obtaining an expression in terms of Z and fundamental constants. How big is this result compared to the ground state energy of hydrogen? How does it compare to hyperfine splitting?

The first-order correction to the ground state energy iis

$$E_0^{(1)} = \int d^3r \psi_0^{*(0)}(\vec{r}) H_1(r) \psi_0^{(0)}(\vec{r}) \quad ,$$
$$\psi_0^{(0)}(\vec{r}) = \sqrt{\frac{\alpha^3}{\pi}} e^{-\alpha r} \, , \quad (\ell = 0) \, , \quad \alpha = \frac{Z}{a_0}$$

Now
$$\frac{R}{a_0} = \frac{r_0}{a_0} A^{1/3} \approx 10^{-5} A^{1/3} << 1$$

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

$$E_0^{(1)} = 4\alpha^3 \int_0^R r^2 dr \left(1 - \frac{2\alpha r}{a_0} + \left(\frac{2\alpha r}{a_0}\right)^2\right) \left(\frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2}\right) + \frac{Ze^2}{r}\right)$$
$$= 4\alpha^3 \left(\begin{array}{c} \left(\frac{Ze^2}{R}\left(\frac{R^5}{10R^2} - \frac{3R^3}{6}\right) + \frac{Ze^2R^2}{2}\right) - \frac{2\alpha}{a_0}\left(\frac{Ze^2}{R}\left(\frac{R^6}{12R^2} - \frac{3R^4}{8}\right)\right) \\ + \frac{Ze^2R^3}{3} + \left(\frac{2\alpha}{a_0}\right)^2 \left(\frac{Ze^2}{R}\left(\frac{R^7}{14R^2} - \frac{3R^5}{10}\right) + \frac{Ze^2R^4}{4}\right) \end{array} \right)$$
$$= 4\alpha^3 \left(\frac{1}{10} Ze^2R^2 - \frac{\alpha}{12a_0} Ze^2R^3 + \frac{3}{140}\left(\frac{2\alpha}{a_0}\right)^2 Ze^2R^4\right)$$
$$\approx \frac{2}{5} Ze^2R^2\alpha^3 = \frac{4}{5}\frac{Z^4e^2}{2a_0}\left(\frac{R}{a_0}\right)^2$$

The effect compared to the ground states energy of hydrogen ($Z = 1$) is

$$\frac{\left|E_0^{(1)}\right|}{\left|E_0^{(0)}\right|} = \frac{\frac{4}{5}\frac{e^2}{2a_0}\left(\frac{R}{a_0}\right)^2}{\frac{e^2}{2a_0}} = \frac{4}{5}\left(\frac{R}{a_0}\right)^2 \approx 10^{-10}$$

This is the same size as the hyperfine splitting due to magnetic moment interactions.

8.9.12 Spin-Oscillator Coupling

Consider a Hamiltonian describing a spin$-1/2$ particle in a harmonic well as given below:

$$\hat{H}_0 = \frac{\hbar\omega}{2}\hat{\sigma}_z + \hbar\omega\left(\hat{a}^+\hat{a} + 1/2\right)$$

(a) Show that

$$\{|n\rangle \otimes |\downarrow\rangle = |n,\downarrow\rangle \ , \ |n\rangle \otimes |\uparrow\rangle = |n,\uparrow\rangle\}$$

are energy eigenstates with eigenvalues $E_{n,\downarrow} = n\hbar\omega$ and $E_{n,\uparrow} = (n+1)\hbar\omega$, respectively.

The basis set is

$$\{|n\rangle \otimes |\uparrow\rangle, |n\rangle \otimes |\downarrow\rangle\} \quad , \quad n = 0, 1, 2, ...$$

where

$$\hat{H}_0 |n\rangle \otimes |\uparrow\rangle = \hbar\omega\left(\hat{a}^+\hat{a} + 1/2\right)|n\rangle \otimes |\uparrow\rangle + \frac{\hbar\omega}{2}\hat{\sigma}_z |n\rangle \otimes |\uparrow\rangle \quad = \left(\hbar\omega\,(n + 1/2) + \frac{\hbar\omega}{2}\right)|n\rangle \otimes |\uparrow\rangle = \hbar\omega$$

and

$$\hat{H}_0 |n\rangle \otimes |\downarrow\rangle = \hbar\omega\left(\hat{a}^+\hat{a} + 1/2\right)|n\rangle \otimes |\downarrow\rangle + \frac{\hbar\omega}{2}\hat{\sigma}_z |n\rangle \otimes |\downarrow\rangle$$
$$= \left(\hbar\omega\,(n + 1/2) - \frac{\hbar\omega}{2}\right)|n\rangle \otimes |\downarrow\rangle = \hbar\omega n\,|n\rangle \otimes |\downarrow\rangle$$

so that $\{|n\rangle \otimes |\uparrow\rangle, |n\rangle \otimes |\downarrow\rangle\} \quad , \quad n = 0, 1, 2, ...$ are eigenstates of $hatH_0$ with eigenvalues $\{\hbar\omega\,(n+1), \hbar\omega n\}$.

(b) The states associated with the ground-state energy and the first excited energy level are

$$\{|0,\downarrow\rangle \ , \ |1,\downarrow\rangle \ , \ |0,\uparrow\rangle\}$$

What is(are) the ground state(s)? What is(are) the first excited state(s)? Note: two states are degenerate.

The ground state is

$$|n = 0,\downarrow\rangle \Rightarrow E_{0,\downarrow} = 0$$

The doubly degenerate first-excited states are

$$|n = 1,\downarrow\rangle \Rightarrow E_{1,\downarrow} = \hbar\omega \quad , \quad |n = 0,\uparrow\rangle \Rightarrow E_{0,\uparrow} = \hbar\omega$$

(c) Now consider adding an interaction between the harmonic motion and the spin, described by the Hamiltonian

$$\hat{H}_1 = \frac{\hbar\Omega}{2}\left(\hat{a}\hat{\sigma}_+ + \hat{a}^+\hat{\sigma}_-\right)$$

so that the total Hamiltonian is now $\hat{H} = \hat{H}_0 + \hat{H}_1$. Write a matrix representation of $\hat{H}$ in the subspace of the ground and first excited states in the ordered basis given in part (b).

We add an interaction

$$\hat{H}_1 = \frac{\hbar\Omega}{2}\left(\hat{a}\hat{\sigma}_+ + \hat{a}^+\hat{\sigma}_-\right)$$

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

$$\begin{aligned}
\hat{H}_1|n=0,\downarrow\rangle &= \tfrac{\hbar\Omega}{2}\left(\hat{a}\hat{\sigma}_+ + \hat{a}^+\hat{\sigma}_-\right)|n=0,\downarrow\rangle = 0 \\
\hat{H}_1|n=1,\downarrow\rangle &= \tfrac{\hbar\Omega}{2}\left(\hat{a}\hat{\sigma}_+ + \hat{a}^+\hat{\sigma}_-\right)|n=1,\downarrow\rangle = \tfrac{\hbar\Omega}{2}|n=0,\uparrow\rangle \\
\hat{H}_1|n=0,\uparrow\rangle &= \tfrac{\hbar\Omega}{2}\left(\hat{a}\hat{\sigma}_+ + \hat{a}^+\hat{\sigma}_-\right)|n=0,\uparrow\rangle = \tfrac{\hbar\Omega}{2}|n=1,\downarrow\rangle
\end{aligned}$$

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 2×2 submatrix and find the eigenvalues from the characteristic equation

$$\det\begin{pmatrix} -\lambda & \frac{\hbar\Omega}{2} \\ \frac{\hbar\Omega}{2} & -\lambda \end{pmatrix} = 0 \Rightarrow \lambda = \pm\frac{\hbar\Omega}{2}$$

so that to first-order

$$E^{(1)}_{\pm} = \pm\frac{\hbar\Omega}{2}$$

The new eigenstates in the first-excited state subspace are

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(|n=0,\uparrow\rangle \pm |n=1,\downarrow\rangle\right)$$

8.9.13 Motion in spin-dependent traps

Consider an electron moving in one dimension, in a spin-dependent trap as shown in Figure 8.4 below:

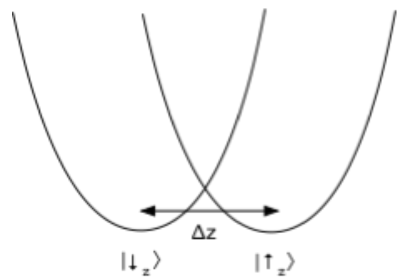


Figure 8.4: A spin-dependent trap

If the electron is in a spin-up state (with respect to the $z-$axis), it is trapped in the right harmonic oscillator well and if it is in a spin-down state (with respect to the $z-$axis), it is trapped in the left harmonic oscillator well. The Hamiltonian that governs its dynamics can be written as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_{osc}^2(\hat{z} - \Delta z/2)^2 \otimes |\uparrow_z\rangle\langle\uparrow_z| + \frac{1}{2}m\omega_{osc}^2(\hat{z} + \Delta z/2)^2 \otimes |\downarrow_z\rangle\langle\downarrow_z|$$

(a) What are the energy levels and stationary states of the system? What are the degeneracies of these states? Sketch an energy level diagram for the first three levels and label the degeneracies.

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

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_{osc}^2(\hat{z} - \Delta z/2)^2 \otimes |\uparrow_z\rangle\langle\uparrow_z| + \frac{1}{2}m\omega_{osc}^2(\hat{z} + \Delta z/2)^2 \otimes |\downarrow_z\rangle\langle\downarrow_z|$$

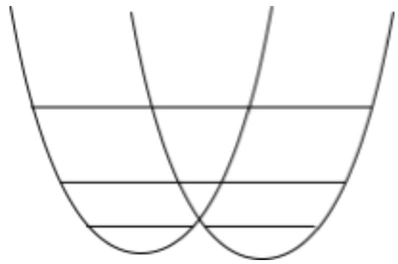
In the absence of coupling(see Hamiltonian) between $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$ there is a doubly degenerate spectrum. The energy levels ar

$$E_n = \hbar\omega\,(n + 1/2) \quad , \quad n = 0, 1, 2, ...$$

each with two distinct spin states $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$. Thus, we have two orthogonal quantum states for each energy level

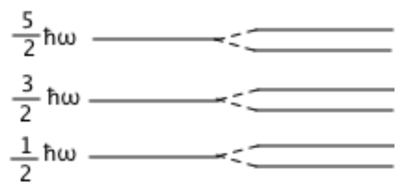
$$|n\rangle_R \otimes |\uparrow_z\rangle \quad , \quad |n\rangle_L \otimes |\downarrow_z\rangle$$

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 $|\mu_B B_x| << \hbar\omega_{osc}$. 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



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

$$|1\rangle = |n\rangle_L \otimes |\downarrow_z\rangle \quad , \quad |2\rangle = |n\rangle_R \otimes |\uparrow_z\rangle$$

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

$$\langle 1|\hat{H}_1|1\rangle = \langle \downarrow_z| \otimes {}_L\langle n| \frac{\hbar\Omega}{2}\hat{\sigma}_x \otimes \hat{I}_{motion} |\downarrow_z\rangle |n\rangle_L$$
$$= \frac{\hbar\Omega}{2} \langle \downarrow_z|\hat{\sigma}_x|\downarrow_z\rangle \, {}_L\langle n|\hat{I}_{motion}|n\rangle_L = 0$$

$$\langle 2|\hat{H}_1|2\rangle = \langle \uparrow_z| \otimes {}_R\langle n| \frac{\hbar\Omega}{2}\hat{\sigma}_x \otimes \hat{I}_{motion} |\uparrow_z\rangle |n\rangle_R$$
$$= \frac{\hbar\Omega}{2} \langle \uparrow_z|\hat{\sigma}_x|\uparrow_z\rangle \, {}_R\langle n|\hat{I}_{motion}|n\rangle_R = 0$$

$$\langle 1|\hat{H}_1|2\rangle = \langle \downarrow_z| \otimes {}_L\langle n| \frac{\hbar\Omega}{2}\hat{\sigma}_x \otimes \hat{I}_{motion} |\uparrow_z\rangle |n\rangle_R$$
$$= \frac{\hbar\Omega}{2} \langle \downarrow_z|\hat{\sigma}_x|\uparrow_z\rangle \, {}_L\langle n|\hat{I}_{motion}|n\rangle_R = \frac{\hbar\Omega}{2}\langle n_L \mid n_R\rangle = \langle 2|\hat{H}_1|1\rangle^*$$
$$\langle 2|\hat{H}_1|1\rangle = \frac{\hbar\Omega}{2}\langle n_L \mid n_R\rangle^* = \frac{\hbar\Omega}{2}\langle n_L \mid n_R\rangle$$

where the last step follows since the motion wavefunctions are real.

Thus,

$$\hat{H}_1 = \begin{pmatrix} 0 & \frac{\hbar\Omega}{2}\langle n_L \mid n_R\rangle \\ \frac{\hbar\Omega}{2}\langle n_L \mid n_R\rangle & 0 \end{pmatrix} = \frac{\hbar\Omega}{2}\langle n_L \mid n_R\rangle \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

as we would expect. The eigenvalues are

$$E_{\pm}^{(1)} = \pm\frac{\hbar\Omega}{2}\langle n_L \mid n_R\rangle$$

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 Δz macroscopic, these are sometimes called Schrodinger cat states. Explain why.

The eigenvectors are entangled states

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|1\rangle \pm |2\rangle) = \frac{1}{\sqrt{2}}(|n\rangle_L \otimes |\downarrow_z\rangle \pm |n\rangle_R \otimes |\uparrow_z\rangle)$$

which are the same as the Schrodinger cat states of the form

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|decay\rangle \otimes |dead\rangle \pm |no\ decay\rangle \otimes |alive\rangle)$$

8.9.14 Perturbed Oscillator

A particle of mass m is moving in the 3−dimensional harmonic oscillator potential

$$V(x,y,z) = \frac{1}{2}m\omega^2(x^2+y^2+z^2)$$

A weak perturbation is applied in the form of the function

$$\Delta V(x,y,z) = kxyz + \frac{k^2}{\hbar\omega}x^2y^2z^2$$

where k is a small constant. Calculate the shift in the ground state energy to *second order* in k. This is *not the same* as second-order perturbation theory!

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

$$|n_x,n_y,n_z\rangle \to E^{(0)}_{n_xn_yn_z} = \hbar\omega\left(n_x+n_y+n_z+3/2\right)$$

and

$$\Delta V = kxyz + \frac{k^2}{\hbar\omega}x^2y^2z^2$$

First-order energy correction: From earlier problems we have

$$\begin{aligned}
\langle n'|\,\hat{x}\,|n\rangle &= \sqrt{\tfrac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right)\\
\langle n'|\,\hat{x}^2\,|n\rangle &= \tfrac{\hbar}{2m\omega}\left(\sqrt{n(n-1)}\delta_{n',n-2} + \sqrt{(n+1)(n+2)}\delta_{n',n+2} + (2n+1)\delta_{n',n}\right)
\end{aligned}$$

Therefore,

$$\begin{aligned}
E^{(1)}_{n_xn_yn_z} &= k\langle n_x,n_y,n_z|\,xyz\,|n_x,n_y,n_z\rangle + \frac{k^2}{\hbar\omega}\langle n_x,n_y,n_z|\,x^2y^2z^2\,|n_x,n_y,n_z\rangle\\
&= k\langle n_x|\,x\,|n_x\rangle\langle n_y|\,y\,|n_y\rangle\langle n_z|\,z\,|n_z\rangle + \frac{k^2}{\hbar\omega}\langle n_x|\,x^2\,|n_x\rangle\langle n_y|\,y^2\,|n_y\rangle\langle n_z|\,z^2\,|n_z\rangle\\
&= \frac{k^2}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^3(2n_x+1)(2n_y+1)(2n_z+1)
\end{aligned}$$

so that for the ground state

$$E^{(1)}_{000} = \frac{k^2}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^3 \to O\left(k^2\right) \text{ which is } 2nd\text{-order in } k$$

Second-order energy correction: We have

$$E^{(2)}_{000} = \sum_{n_x,n_y,n_z\neq 0}\frac{\left|\langle n_x,n_y,n_z|\,\Delta V\,|n_x,n_y,n_z\rangle\right|^2}{E^{(0)}_{000} - E_{n_xn_yn_z}}$$

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,

$$\begin{aligned}E_{000}^{(2)} &= k^2 \sum_{n_x,n_y,n_z\neq 0} \frac{\left|\langle n_x, n_y, n_z| \, xyz \, |0,0,0\rangle\right|^2}{3\hbar\omega/2 - \hbar\omega\left(n_x+n_y+n_z+3/2\right)} \\ &= -k^2 \sum_{n_x,n_y,n_z\neq 0} \frac{\left|\langle n_x| \, x \, |0\rangle \langle n_y| \, y \, |0\rangle \langle n_z| \, z \, |0\rangle\right|^2}{\hbar\omega\left(n_x+n_y+n_z\right)}\end{aligned}$$

Now,

$$\langle n_x| \, x \, |0\rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n_x| \left(\hat{a}+\hat{a}^+\right) |0\rangle = \sqrt{\frac{\hbar}{2m\omega}} \delta_{n_x,1}$$

Therefore,

$$\begin{aligned}E_{000}^{(2)} &= -k^2 \sum_{n_x,n_y,n_z\neq 0} \frac{\left|\langle n_x| \, x \, |0\rangle \langle n_y| \, y \, |0\rangle \langle n_z| \, z \, |0\rangle\right|^2}{\hbar\omega\left(n_x+n_y+n_z\right)} \\ &= -k^2 \left(\frac{\hbar}{2m\omega}\right)^3 \frac{1}{3\hbar\omega} = -\frac{1}{3}\left(\frac{\hbar}{2m\omega}\right)^3 \frac{k^2}{\hbar\omega}\end{aligned}$$

and the energy shift to $2nd$–order ($O(k^2)$) is

$$\Delta E = E_{000}^{(1)} + E_{000}^{(2)} = \frac{2}{3}\left(\frac{\hbar}{2m\omega}\right)^3 \frac{k^2}{\hbar\omega}$$

8.9.15 Another Perturbed Oscillator

Consider the system described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2\alpha}(1 - e^{-\alpha x^2})$$

Assume that $\alpha << m\omega/\hbar$

(1) Calculate an approximate value for the ground state energy using first-order perturbation theory by perturbing the harmonic oscillator Hamiltonian

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

We have

$$\begin{aligned}H &= \tfrac{p^2}{2m} + \tfrac{m\omega^2}{2\alpha}(1-e^{-\alpha x^2}) = H_0 + V \\ H_0 &= \tfrac{p^2}{2m} + \tfrac{m\omega^2}{2}x^2 \Rightarrow V = \tfrac{m\omega^2}{2\alpha}(1-e^{-\alpha x^2}) - \tfrac{m\omega^2}{2}x^2 \\ V &= \tfrac{m\omega^2}{2\alpha}(1-e^{-\alpha x^2}) - \tfrac{m\omega^2}{2}x^2 = \tfrac{m\omega^2}{2}\left[\tfrac{1-e^{-\alpha x^2}}{\alpha} - x^2\right]\end{aligned}$$

The normalized unperturbed ground state energy eigenfunction of the unperturbed harmonic oscillator is

$$\varphi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\left(\frac{m\omega}{2\hbar}\right)x^2}$$

Thus, the first-order correction to the ground-state energy is

$$\langle\varphi_0|\,V\,|\varphi_0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\frac{m\omega^2}{2}\int\limits_{-\infty}^{\infty} dx e^{-\left(\frac{m\omega}{\hbar}\right)x^2}\left[\frac{1-e^{-\alpha x^2}}{\alpha}-x^2\right]$$

Now

$$\int\limits_0^{\infty} x^n e^{-\lambda x^2}dx = \tfrac{1}{2}\frac{\Gamma\left(\frac{n+1}{2}\right)}{\lambda^{\frac{n+1}{2}}}$$
$$\Gamma(x+1) = x\Gamma(x) \quad , \quad \Gamma(1) = 1 \quad , \quad \Gamma(1/2) = \sqrt{\pi}$$

so that

$$\begin{aligned}\langle\varphi_0|\,V\,|\varphi_0\rangle &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\frac{m\omega^2}{2}\int\limits_{-\infty}^{\infty} dx e^{-\left(\frac{m\omega}{\hbar}\right)x^2}\left[\frac{1-e^{-\alpha x^2}}{\alpha}-x^2\right]\\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\frac{m\omega^2}{2}\left(\frac{1}{\alpha}\int\limits_{-\infty}^{\infty} dx e^{-\left(\frac{m\omega}{\hbar}\right)x^2} - \frac{1}{\alpha}\int\limits_{-\infty}^{\infty} dx e^{-\left(\frac{m\omega}{\hbar}+\alpha\right)x^2} - \int\limits_{-\infty}^{\infty} dx x^2 e^{-\left(\frac{m\omega}{\hbar}\right)x^2}\right)\\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\frac{m\omega^2}{2}\left(\begin{array}{l}\frac{1}{\alpha}2\frac{1}{2}\frac{1}{\sqrt{\frac{m\omega}{\hbar}}}\Gamma(1/2)\\ \qquad -\frac{1}{\alpha}\frac{1}{\sqrt{\frac{m\omega}{\hbar}+\alpha}}2\frac{1}{2}\Gamma(1/2) - 2\frac{1}{2}\frac{\Gamma(3/2)}{\left(\frac{m\omega}{\hbar}\right)^{3/2}}\end{array}\right)\\ &= \left(\frac{m\omega}{\hbar}\right)^{1/2}\frac{m\omega^2}{2}\left(\frac{1}{\alpha}\frac{1}{\sqrt{\frac{m\omega}{\hbar}}} - \frac{1}{\alpha}\frac{1}{\sqrt{\frac{m\omega}{\hbar}+\alpha}} - \frac{1}{2}\frac{1}{\left(\frac{m\omega}{\hbar}\right)^{3/2}}\right)\\ &= \frac{m\omega^2}{2\alpha} - \frac{\hbar\omega}{4} - \frac{m\omega^2}{2\alpha}\frac{1}{\sqrt{1+\frac{\alpha\hbar}{m\omega}}} = \frac{m\omega^2}{2\alpha}\left[1-\frac{1}{\sqrt{1+\frac{\alpha\hbar}{m\omega}}}\right] - \frac{\hbar\omega}{4}\end{aligned}$$

Therefore the ground state energy is

$$\begin{aligned}E_0 = E_0^{(0)} + \langle\varphi_0|\,V\,|\varphi_0\rangle &= \frac{\hbar\omega}{2} + \frac{m\omega^2}{2\alpha}\left[1-\frac{1}{\sqrt{1+\frac{\alpha\hbar}{m\omega}}}\right] - \frac{\hbar\omega}{4}\\ &= \hbar\omega\left[\frac{1}{4} + \frac{m\omega}{2\alpha\hbar}\left[1-\frac{1}{\sqrt{1+\frac{\alpha\hbar}{m\omega}}}\right]\right]\end{aligned}$$

(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

$$\langle H \rangle = \frac{\int\limits_{-\infty}^{\infty} e^{-\beta x^2/2}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2\alpha}(1 - e^{-\alpha x^2})\right] e^{-\beta x^2/2} dx}{\int\limits_{-\infty}^{\infty} e^{-\beta x^2} dx}$$

$$= \hbar\omega\left[\frac{1}{4}\left(\frac{\beta\hbar}{m\omega}\right) + \frac{m\omega}{2\hbar\alpha}\left(1 - \frac{1}{\sqrt{1+\alpha/\beta}}\right)\right]$$

To find the value of β that minimizes the energy we set

$$\frac{d\langle H \rangle}{d\beta} = 0$$

We get

$$\frac{d\langle H \rangle}{d\beta} = 0 = \frac{\hbar^2}{4m} - \frac{m\omega^2}{4\beta^2}\frac{1}{(1+\alpha/\beta)^{3/2}}$$
$$\beta\left(1+\alpha/\beta\right)^{3/4} = \frac{m\omega}{\hbar}$$

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

$$\beta\left(1 + \frac{\alpha}{\left(\frac{m\omega}{\hbar}\right)}\right)^{3/4} = \frac{m\omega}{\hbar} \Rightarrow \beta = \frac{m\omega}{\hbar}\left(1 + \frac{\alpha\hbar}{m\omega}\right)^{-3/4}$$

This gives a somewhat smaller value of β and a somewhat lower estimate (and thus better) for $\langle H \rangle$.

8.9.16 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

$$\varphi(\vec{r}_1, \vec{r}_2) = \psi_{100}(r_1)\psi_{100}(r_2)$$
$$\psi_{100}(r) = \sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Zr/a_0} \quad , \quad a_0 = \frac{\hbar^2}{me^2}$$

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

$$E^{(1)} = \langle\varphi| V |\varphi\rangle = e^2 \int\int \frac{d^3\vec{r}_1 d^3\vec{r}_2}{|\vec{r}_1 - \vec{r}_2|} |\psi_{100}(r_1)|^2 |\psi_{100}(r_2)|^2$$
$$= e^2 \left(\frac{Z^3}{\pi a_0^3}\right)^2 \int\int \frac{d^3\vec{r}_1 d^3\vec{r}_2}{|\vec{r}_1 - \vec{r}_2|} e^{-Z(r_1+r_2)/a_0} = e^2 \left(\frac{Z^3}{\pi a_0^3}\right)^2 \frac{20\pi^2}{\left(\frac{2Z}{a_0}\right)^5} = \frac{5Ze^2}{8a_0}$$

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 λ 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

$$E(\lambda) = \langle\varphi| H |\varphi\rangle$$
$$= \int\int d^3\vec{r}_1 d^3\vec{r}_2 e^{-\lambda(r_1+r_2)} \frac{\lambda^3}{\pi} \left(-\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}\right) \frac{\lambda^3}{\pi} e^{-\lambda(r_1+r_2)}$$

Now

$$\begin{aligned}
&\left(\frac{\lambda^3}{\pi}\right)\int d^3\vec{r}_1 e^{-\lambda r_1}\left(-\frac{\hbar^2}{2m}\nabla_1^2-\frac{Ze^2}{r_1}\right)e^{-\lambda r_1}\\
&\quad=\left(\frac{\lambda^3}{\pi}\right)\int d^3\vec{r}_1 e^{-2\lambda r_1}\left(-\frac{\hbar^2}{2m}\frac{1}{r_1^2}\frac{d}{dr_1}\left(r_1^2\frac{d}{dr_1}\right)-\frac{Ze^2}{r_1}\right)e^{-\lambda r_1}\\
&\quad=\left(\frac{\lambda^3}{\pi}\right)\int d^3\vec{r}_1 e^{-2\lambda r_1}\left(-\frac{\hbar^2}{2m}\left(\lambda^2-\frac{2\lambda}{r_1}\right)-\frac{Ze^2}{r_1}\right)e^{-\lambda r_1}\\
&\quad=\left(\frac{\lambda^3}{\pi}\right)\int d^3\vec{r}_1 e^{-2\lambda r_1}\left(-\frac{\hbar^2}{2m}\left(\lambda^2-\frac{2\lambda}{r_1}\right)-\frac{Ze^2+\frac{\hbar^2\lambda}{m}}{r_1}\right)e^{-\lambda r_1}\\
&\quad=-\frac{\hbar^2\lambda^2}{2m}-\left(\frac{\lambda^3}{\pi}\right)\int d^3\vec{r}_1 e^{-2\lambda r_1}\left(\frac{Ze^2+\frac{\hbar^2\lambda}{m}}{r_1}\right)\\
&\quad=-\frac{\hbar^2\lambda^2}{2m}-4\pi\left(\frac{\lambda^3}{\pi}\right)\left(Ze^2+\frac{\hbar^2\lambda}{m}\right)\int r_1 dr_1 e^{-2\lambda r_1}\\
&\quad=-\frac{\hbar^2\lambda^2}{2m}-4\pi\left(\frac{\lambda^3}{\pi}\right)\left(Ze^2+\frac{\hbar^2\lambda}{m}\right)\frac{1}{4\lambda^2}=\frac{\hbar^2\lambda^2}{2m}-Ze^2\lambda
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\int\int d^3\vec{r}_1 d^3\vec{r}_2\frac{\lambda^3}{\pi}e^{-\lambda(r_1+r_2)}\left(-\frac{\hbar^2}{2m}\left(\nabla_1^2+\nabla_2^2\right)-\frac{Ze^2}{r_1}-\frac{Ze^2}{r_2}\right)\frac{\lambda^3}{\pi}e^{-\lambda(r_1+r_2)}\\
&\quad=2\left(\frac{\hbar^2\lambda^2}{2m}-Ze^2\lambda\right)
\end{aligned}$$

and

$$\begin{aligned}
E(\lambda)&=\frac{\hbar^2\lambda^2}{m}-2Ze^2\lambda+\int\int d^3\vec{r}_1 d^3\vec{r}_2\frac{\lambda^3}{\pi}e^{-\lambda(r_1+r_2)}\left(\frac{e^2}{|\vec{r}_1-\vec{r}_2|}\right)\frac{\lambda^3}{\pi}e^{-\lambda(r_1+r_2)}\\
&=\frac{\hbar^2\lambda^2}{m}-2Ze^2\lambda+\frac{\lambda^6}{\pi^2}\frac{20e^2\pi^2}{(2\lambda)^5}=\frac{\hbar^2\lambda^2}{m}-2Ze^2\lambda+\frac{5}{8}e^2\lambda\\
&=\frac{\hbar^2\lambda^2}{m}-\left(2Ze^2-\frac{5}{8}e^2\right)\lambda
\end{aligned}$$

We now find the minimum with respect to λ.

$$\frac{dE(\lambda)}{d\lambda}=0=\frac{d}{d\lambda}\left(\frac{\hbar^2\lambda^2}{m}-\left(2Ze^2-\frac{5}{8}e^2\right)\lambda\right)$$

or

$$\lambda=\frac{me^2}{2\hbar^2}\left(2Z-\frac{5}{8}\right)$$

Therefore, the ground-state energy(for $Z=2$) is

$$E=-\left(Z-\frac{5}{16}\right)^2\frac{me^4}{\hbar^2}=-\left(\frac{27}{16}\right)^2\frac{e^2}{a_0}$$

(c) Compare (a) and (b) with the experimental ionization energy

$$E_{ion} = 1.807 E_0 \quad , \quad E_0 = \frac{\alpha^2 mc^2}{2} \quad , \quad \alpha = \text{ fine structure constant}$$

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

$$\psi_{1s}(r) = \sqrt{\frac{\lambda^3}{\pi}} \exp(-\lambda r) \quad , \quad a_0 = \frac{\hbar^2}{me^2} \quad , \quad \int\int d^3r_1 d^3r_2 \frac{e^{-\beta(r_1+r_2)}}{|\vec{r}_1 - \vec{r}_2|} = \frac{20\pi^2}{\beta^5}$$

That last integral is very hard to evaluate from first principles.

8.9.17 Hydrogen atom + xy perturbation

An electron moves in a Coulomb field centered at the origin of coordinates. The first excited state ($n = 2$) is 4−fold degenerate. Consider what happens in the presence of a non-central perturbation

$$V_{pert} = f(r)xy$$

where $f(r)$ is some function only of r, which falls off rapidly as $r \to \infty$. To first order, this perturbation splits the 4−fold degenerate level into several distinct levels (some might still be degenerate).

(a) How many levels are there?

(b) What is the degeneracy of each?

(c) Given the energy shift, call it ΔE, for one of the levels, what are the values of the shifts for all the others?

The four degenerate unperturbed wave functions are

$$\begin{aligned}
\langle \vec{r} \mid 2,0,0\rangle &= R_{20}(r) Y_{0,0}(\theta,\phi) \\
\langle \vec{r} \mid 2,1,1\rangle &= R_{21}(r) Y_{1,1}(\theta,\phi) \\
\langle \vec{r} \mid 2,1,0\rangle &= R_{21}(r) Y_{1,0}(\theta,\phi) \\
\langle \vec{r} \mid 2,1,-1\rangle &= R_{21}(r) Y_{1,-1}(\theta,\phi)
\end{aligned}$$

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 4×4 degenerate submatrix for the perturbation

$$V = f(r)xy = f(r) r^2 \sin^2\theta \sin\phi \cos\phi$$

with matrix elements

$$\begin{aligned} V_{\ell' m';\ell m} &= \langle \ell' m' | \hat{V} | \ell m \rangle \\ &= \int R_{2\ell'}(r) R_{2\ell}(r) r^4 f(r) dr \int Y^*_{\ell' m'}(\theta,\phi) Y_{\ell m}(\theta,\phi) \sin^3\theta \sin\phi \cos\phi d\theta d\phi \end{aligned}$$

The necessary spherical harmonics are

$$\begin{array}{ll} Y_{0,0} = \frac{1}{\sqrt{4\pi}} \quad , & Y_{1,1} = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{i\phi} \\ Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta \quad , & Y_{1,-1} = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{-i\phi} \end{array}$$

Now the ϕ 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

$$m = 1 = -m' \quad or \quad m = -1 = -m'$$

Therefore, the only nonzero matrix elements are

$$\begin{aligned} V_{1,-1;1,1} &= V^*_{1,1;1,-1} \\ &= \int R_{21}(r) R_{21}(r) r^4 f(r) dr \int Y^*_{1,-1}(\theta,\phi) Y_{11}(\theta,\phi) \sin^3\theta \sin\phi \cos\phi d\theta d\phi \\ &= \frac{3}{8\pi} \int_0^\infty R^2_{21}(r) r^4 f(r) dr \int_0^\pi \sin^5\theta d\theta \int_0^{2\pi} \sin\phi \cos\phi e^{-2i\phi} d\phi = iA \end{aligned}$$

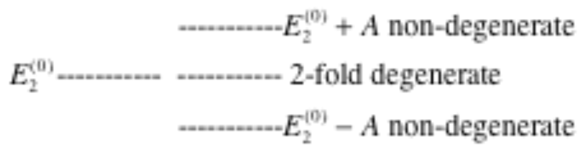
where

$$A = \frac{1}{5} \int_0^\infty R^2_{21}(r) r^4 f(r) dr$$

Therefore the V matrix look like

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & iA \\ 0 & 0 & -iA & 0 \end{pmatrix} \rightarrow eigenvalues = 0, 0, \pm A$$

Therefore the original 4-fold degenerate level splits into three new levels with the remaining degeneracy as indicated.



8.9.18 Rigid rotator in a magnetic field

Suppose that the Hamiltonian of a rigid rotator in a magnetic field is of the form

$$\hat{H} = A\vec{L}^2 + B\hat{L}_z + C\hat{L}_y$$

Assuming that $A\,,\,B \gg C$, use perturbation theory to lowest nonvanishing order to get approximate energy eigenvalues.

We have

$$\hat{H} = A\hat{\vec{L}}^2 + B\hat{L}_z + C\hat{L}_y$$

We choose the unperturbed basis states $|L, M\rangle$ where

$$\begin{aligned}\hat{L}^2 \,|L, M\rangle &= \hbar^2 L(L+1)\,|L, M\rangle \\ \hat{L}_z \,|L, M\rangle &= M\hbar\,|L, M\rangle\end{aligned}$$

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

$$\hat{H}_0 = A\hat{\vec{L}}^2 + B\hat{L}_z \quad , \quad \hat{V} = C\hat{L}_y = C\frac{\hat{L}_+ - \hat{L}_-}{2i}$$

The unperturbed energies are given by

$$\begin{aligned}\hat{H}_0\,|L, M\rangle &= A\hat{\vec{L}}^2\,|L, M\rangle + B\hat{L}_z\,|L, M\rangle \\ &= \left(A\hbar^2 L(L+1) + BM\hbar\right)|L, M\rangle = E^{(0)}_{LM}\,|L, M\rangle\end{aligned}$$

These levels are non-degenerate.

The general matrix element of $\hat{V}$ is given by

$$\begin{aligned}\langle L'M'|\,\hat{V}\,|LM\rangle &= \frac{C}{2i}\left(\langle L'M'|\,\hat{L}_+\,|LM\rangle - \langle L'M'|\,\hat{L}_-\,|LM\rangle\right) \\ &= \frac{C\hbar}{2i}\left(\begin{array}{c}\sqrt{L(L+1) - M(M+1)}\delta_{L'L}\delta_{M',M+1} \\ -\sqrt{L(L+1) - M(M-1)}\delta_{L'L}\delta_{M',M-1}\end{array}\right)\end{aligned}$$

Since the diagonal matrix elements are zero, we have no first-order corrections, that is, $E_{LM}^{(1)} = 0$.

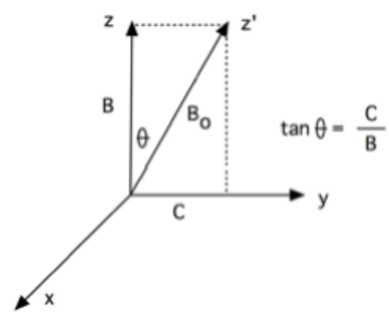
The second-order corrections (non-degenerate levels) are given by

$$E_{LM}^{(2)} = \frac{C^2\hbar^2}{4} \sum_{M' \neq M} \frac{\left|\sqrt{L(L+1)-M(M+1)}\delta_{L'L}\delta_{M',M+1} - \sqrt{L(L+1)-M(M-1)}\delta_{L'L}\delta_{M',M-1}\right|^2}{E_{LM}^{(0)} - E_{LM'}^{(0)}}$$
$$= \frac{C^2\hbar^2}{4}\left(\frac{L(L+1)-M(M+1)}{-B\hbar} + \frac{L(L+1)-M(M-1)}{B\hbar}\right)$$
$$= \frac{C^2\hbar}{4B}\left(M(M+1)-M(M-1)\right) = \frac{C^2\hbar}{2B}M$$

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

$$\hat{H} = A\hat{L}^2 + B_0\hat{L}_{z'} \quad , \quad B_0 = \sqrt{B^2 + C^2}$$

We can solve this problem exactly. We get

$$E = A\hbar^2 L(L+1) + \left(B^2 + C^2\right)^2 M'\hbar$$

where

$$|L, M'\rangle = D\left(\frac{\pi}{2}, 0, 0\right)|L, M\rangle = \sum_{M=-L}^{L} D_{MM'}^{(L)}\left(\frac{\pi}{2}, 0, 0\right)|L, M\rangle$$

For $B \gg C$ we have

$$E = A\hbar^2 L(L+1) + BM'\hbar + \frac{C^2}{2B}M'\hbar \quad , \quad M' \approx M$$

which is the same result as above.

8.9.19 Another rigid rotator in an electric field

Consider a rigid body with moment of inertia I, which is constrained to rotate in the $xy-$plane, and whose Hamiltonian is

$$\hat{H} = \frac{1}{2I}\hat{L}_z^2$$

Find the eigenfunctions and eigenvalues (zeroth order solution). Now assume the rotator has a fixed dipole moment $\vec{p}$ in the plane. An electric field $\vec{\mathcal{E}}$ is applied in the plane. Find the change in the energy levels to first and second order in the field.

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 θ 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

$$-\frac{\hbar^2}{2I}\frac{d^2\psi}{d\theta^2} = E\psi$$

which has solutions

$$\psi_m(\theta) = \frac{1}{\sqrt{2\pi}}e^{im\theta} \quad , \quad m = 0, \pm 1, \pm 2, ...$$

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

$$V = -\vec{p}\cdot\vec{\varepsilon} = -p\varepsilon\cos\theta$$

The first-order energy correction is

$$E_m^{(1)} = \langle m| V |m\rangle = -\frac{p\varepsilon}{2\pi}\int_0^{2\pi}\cos\theta d\theta = 0$$

The second-order correction is

$$E_m^{(2)} = \sum_{m'\neq m}\frac{\left|\langle m'| V |m\rangle\right|^2}{E_m^{(0)} - E_{m'}^{(0)}}$$

Since

$$\langle m'| V |m\rangle = -\frac{p\varepsilon}{2\pi}\int\limits_0^{2\pi} e^{i(m-m')\theta}\cos\theta d\theta = -\frac{p\varepsilon}{4\pi}\int\limits_0^{2\pi} (e^{i(m-m'+1)\theta} + e^{i(m-m'-1)\theta})d\theta$$
$$= -\frac{p\varepsilon}{2}\left(\delta_{m',m+1} + \delta_{m',m-1}\right)$$

we have for $m \neq 0$

$$E_m^{(2)} = \frac{p^2\varepsilon^2}{4}\frac{2I}{\hbar^2}\left(\frac{1}{m^2-(m-1)^2} + \frac{1}{m^2-(m+1)^2}\right)$$
$$= \frac{p^2\varepsilon^2 I}{\hbar^2}\frac{1}{4m^2-1}$$

If $m = 0$, only the first term $\delta_{m',m+1}$ is valid and we get

$$E_0^{(2)} = -\frac{p^2\varepsilon^2 I}{2\hbar^2}$$

8.9.20 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

$$\hat{H}_0 |S, M\rangle = \alpha(\hat{S}^2 - 2\hat{S}_z^2)/\hbar^2 |S, M\rangle = \alpha\left(S(S+1) - 2M^2\right)|S, M\rangle$$

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 trip;ly degenerate, and 2α, which is non-degenerate or simple.

The corresponding eigenvectors are

$$|1,1\rangle = |1/2\rangle_1 |1/2\rangle_2$$
$$|1,0\rangle = \tfrac{1}{\sqrt{2}}\left(|1/2\rangle_1 |-1/2\rangle_2 + |-1/2\rangle_1 |1/2\rangle_2\right)$$
$$|1,-1\rangle = |-1/2\rangle_1 |-1/2\rangle_2$$
$$|0,0\rangle = \tfrac{1}{\sqrt{2}}\left(|1/2\rangle_1 |-1/2\rangle_2 - |-1/2\rangle_1 |1/2\rangle_2\right)$$

(b) Consider the perturbation $\hat{H}_1 = \lambda(\hat{S}_{1x} - \hat{S}_{2x})$. Calculate the new energies in first-order perturbation theory.

Since

$$\hat{S}_x |1/2\rangle = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}|-1/2\rangle$$

and similarly,

$$\hat{S}_x |-1/2\rangle = \frac{\hbar}{2}|1/2\rangle$$

it then follows that

$$\begin{aligned}\hat{H}_1 |1,1\rangle &= \lambda(\hat{S}_{1x} - \hat{S}_{2x})|1,1\rangle = \lambda(\hat{S}_{1x} - \hat{S}_{2x})|1/2\rangle_1 |1/2\rangle_2 \\ &= \frac{\lambda\hbar}{2}\left(|-1/2\rangle_1 |1/2\rangle_2 - |1/2\rangle_1 |-1/2\rangle_2\right) = -\frac{\lambda\hbar}{\sqrt{2}}|0,0\rangle\end{aligned}$$

and similarly,

$$\begin{aligned}\hat{H}_1 |1,0\rangle &= \lambda(\hat{S}_{1x} - \hat{S}_{2x})|1,0\rangle \\ &= \lambda(\hat{S}_{1x} - \hat{S}_{2x})\frac{1}{\sqrt{2}}\left(|1/2\rangle_1 |-1/2\rangle_2 + |-1/2\rangle_1 |1/2\rangle_2\right) = 0\end{aligned}$$

and

$$\begin{aligned}\hat{H}_1 |1,-1\rangle &= \lambda(\hat{S}_{1x} - \hat{S}_{2x})|1,-1\rangle \\ &= \lambda(\hat{S}_{1x} - \hat{S}_{2x})|-1/2\rangle_1 |-1/2\rangle_2 = \frac{\lambda\hbar}{\sqrt{2}}|0,0\rangle\end{aligned}$$

Therefore, $\langle 1,0|\hat{H}_1|1,0\rangle = 0$, which means that the eigenvector, $|1,0\rangle$, of energy 2α, 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 characterisitic equation

$$\begin{vmatrix} -E & -\frac{\lambda\hbar}{\sqrt{2}} & 0 \\ -\frac{\lambda\hbar}{\sqrt{2}} & -E & \frac{\lambda\hbar}{\sqrt{2}} \\ 0 & \frac{\lambda\hbar}{\sqrt{2}} & -E \end{vmatrix} = 0 = -E(E^2 - \lambda^2\hbar^2) \to E = 0,\ \pm\lambda\hbar$$

Therefore, the energy levels are shifted in this way:

$0(3-fold) \Rightarrow 0,\ \pm\lambda\hbar$ (no remaining degeneracy)
$2\alpha \Rightarrow 2\alpha$ (unshifted)

8.9.21 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

$$\begin{array}{lll} \hat{H}_0 = -A(\hat{S}_{1z} + \hat{S}_{2z}) & & \\ |{+}{+}\rangle & , & -A\hbar \\ |{+}{-}\rangle & , & 0 \\ |{-}{-}\rangle & , & A\hbar \\ |{-}{+}\rangle & , & 0 \end{array}$$

(b) Calculate the exact eigenvalues of $\hat{H}_0 + \hat{H}_1$

We can rewrite the perturbation as

$$\hat{H}_1 = B(\hat{S}_{1x}\hat{S}_{2x} - \hat{S}_{1y}\hat{S}_{2y}) = B\left(\frac{\hat{S}_{1+} + \hat{S}_{1-}}{2}\frac{\hat{S}_{2+} + \hat{S}_{2-}}{2} - \frac{\hat{S}_{1+} - \hat{S}_{1-}}{2i}\frac{\hat{S}_{2+} - \hat{S}_{2-}}{2i}\right)$$
$$= \frac{1}{2}B\left(\hat{S}_{1+}\hat{S}_{2+} + \hat{S}_{1-}\hat{S}_{2-}\right)$$

We then have

$$\begin{array}{l} \hat{H}_1 |{+}{+}\rangle = \frac{1}{2}B\left(\hat{S}_{1+}\hat{S}_{2+} + \hat{S}_{1-}\hat{S}_{2-}\right)|{+}{+}\rangle = \frac{1}{2}B\hat{S}_{1-}\hat{S}_{2-}|{+}{+}\rangle = \frac{1}{2}B\hbar^2|{-}{-}\rangle \\ \hat{H}_1 |{-}{-}\rangle = \frac{1}{2}B\hbar^2|{+}{+}\rangle \\ \hat{H}_1 |{-}{+}\rangle = 0 \\ \hat{H}_1 |{+}{-}\rangle = 0 \end{array}$$

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

$$\frac{1}{\sqrt{2}}\left(|{+}{-}\rangle \pm |{-}{+}\rangle\right)$$

To obtain the other eigenvectors, consider the eigenvalue equation

$$(\hat{H}_0 + \hat{H}_1)\left(\cos\theta\,|{+}{+}\rangle + \sin\theta\,|{-}{-}\rangle\right) = \lambda\left(\cos\theta\,|{+}{+}\rangle + \sin\theta\,|{-}{-}\rangle\right)$$

and

$$-A\hbar\left(\cos\theta\,|{+}{+}\rangle - \sin\theta\,|{-}{-}\rangle\right) + \frac{1}{2}B\hbar^2\left(\cos\theta\,|{-}{-}\rangle + \sin\theta\,|{+}{+}\rangle\right) = \lambda\left(\cos\theta\,|{+}{+}\rangle + \sin\theta\,|{-}{-}\rangle\right)$$

We then have

$$\begin{array}{l} -A\hbar\cos\theta + \frac{1}{2}B\hbar^2\sin\theta = \lambda\cos\theta \rightarrow (A\hbar + \lambda)\cos\theta = \frac{1}{2}B\hbar^2\sin\theta \\ A\hbar\sin\theta + \frac{1}{2}B\hbar^2\cos\theta = \lambda\sin\theta \rightarrow (-A\hbar + \lambda)\sin\theta = \frac{1}{2}B\hbar^2\cos\theta \end{array}$$

or

$$\frac{(A\hbar+\lambda)}{\frac{1}{2}B\hbar^2} = \frac{\frac{1}{2}B\hbar^2}{(-A\hbar+\lambda)} \to \lambda^2 - A^2\hbar^2 = \frac{1}{4}B^2\hbar^4 \to \lambda = \pm\frac{\hbar}{2}\sqrt{4A^2+B^2\hbar^2}$$

Now

$$\lambda_- = -\frac{\hbar}{2}\sqrt{4A^2+B^2\hbar^2}$$

corresponds to the ground state and we find the eigenvector as follows. We have

$$\frac{(A\hbar+\lambda_-)}{B\hbar^2/2} = \tan\theta = \frac{(A\hbar - \frac{\hbar}{2}\sqrt{4A^2+B^2\hbar^2})}{B\hbar^2/2}$$

and

$$\begin{aligned} \left|\lambda_-\right\rangle &= \cos\theta\left|--\right\rangle + \sin\theta\left|++\right\rangle = C\left(\left|--\right\rangle + \tan\theta\left|++\right\rangle\right) \\ &= C\left(\left|--\right\rangle + \tan\theta\left|++\right\rangle\right) \end{aligned}$$

Similarly,

$$\lambda + = +\frac{\hbar}{2}\sqrt{4A^2+B^2\hbar^2}$$

corresponds to the highest energy state and

$$\frac{(A\hbar+\lambda_+)}{B\hbar^2/2} = \tan\theta = \frac{(A\hbar + \frac{\hbar}{2}\sqrt{4A^2+B^2\hbar^2})}{B\hbar^2/2}$$

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

$$\left\langle ++\right|\hat{H}_1\left|++\right\rangle = \left\langle +-\right|\hat{H}_1\left|+-\right\rangle = \left\langle -+\right|\hat{H}_1\left|-+\right\rangle = \left\langle --\right|\hat{H}_1\left|--\right\rangle = 0$$

so that the first order correction to the energy is zero. For the ground state, $\left|+,+\right\rangle$ with unperturbed energy $-A\hbar$, the only contribution in second-order comes from the term

$$\left\langle --\right|\hat{H}_1\left|++\right\rangle = \frac{1}{2}B\hbar^2$$

and so, to second-order in B, the ground state energy is

$$-A\hbar + \frac{\left|\left\langle --\right|\hat{H}_1\left|++\right\rangle\right|^2}{(-A\hbar)-(A\hbar)} = -A\hbar - \frac{B^2\hbar^3}{8A}$$

The exact energy is

$$\lambda_- = -\frac{\hbar}{2}\sqrt{4A^2+B^2\hbar^2}$$

which corresponds (for $A \gg B$) to

$$\lambda_- = -A\hbar\sqrt{1+\frac{B^2\hbar^2}{4A^2}} \approx -A\hbar\left(1+\frac{B^2\hbar^2}{8A^2}\right) = -A\hbar - \frac{B^2\hbar^3}{8A}$$

which agrees with the second-order result.

8.9.22 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 Schrodinger equation for the particle in the potential well is

$$R'' + \frac{2}{r}R' + \left(k^2 - \frac{\ell(\ell+1)}{r^2}\right)R = 0 \quad , \quad E = \frac{\hbar^2 k^2}{2m}$$

The boundary condition is $R(r-R) = 0$. Introducing a dimensionless variable $\rho = kr$, we get

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left(1 - \frac{\ell(\ell+1)}{\rho^2}\right)R = 0$$

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

$$R_{k\ell}(r) = C_{kl} j_\ell(kr) \quad , \quad C_{kl} = \text{ normalization factor}$$

The boundary condition requires that

$$j_\ell(kR) = 0$$

which has solutions

$$kR = \alpha_{n\ell} \quad , \quad n = 1, 2, ...$$

where the $\alpha_{n\ell}$ is the n^{th} zero of the ℓ^{th} order spherical Bessel function. Then the bound states of the particle have energies given by

$$E_{n\ell} = \frac{\hbar^2}{2mR^2}\alpha_{n\ell}^2 \quad , \quad n = 1, 2, ...$$

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 cab be written

$$A_x = -\frac{By}{2} \quad , \quad A_y = \frac{Bx}{2} \quad , \quad A_z = 0$$

and

$$\begin{aligned}
\hat{H} &= \frac{1}{2m}\left(\left(\hat{p}_x + \frac{eB}{2c}\hat{y}\right)^2 + \left(\hat{p}_y - \frac{eB}{2c}\hat{x}\right)^2 + \hat{p}_z^2\right) + V(r) \\
&= \frac{1}{2m}\left(\vec{p}^2 - \frac{eB}{c}\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right) + \frac{e^2B^2}{4c^2}\left(\hat{x}^2 + \hat{y}^2\right)\right) + V(r) \\
&= \frac{1}{2m}\left(\vec{p}^2 - \frac{eB}{c}\hat{L}_z + \frac{e^2B^2}{4c^2}\left(\hat{x}^2 + \hat{y}^2\right)\right) + V(r)
\end{aligned}$$

Since the magnetic field is weak, we can treat the term

$$-\frac{eB}{c}\hat{L}_z + \frac{e^2B^2}{4c^2}\left(\hat{x}^2 + \hat{y}^2\right)$$

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

$$\frac{e^2B^2}{4c^2}\left(\hat{x}^2 + \hat{y}^2\right) = \frac{e^2B^2}{4c^2}r^2\sin^2\theta$$

The ground state wave function is

$$\psi(r,\theta,\phi) = j_0(kr)Y_{00} = \frac{C}{\sqrt{4\pi}}\frac{\sin kr}{kr}$$

Normalizing we have

$$1 = C^2\frac{1}{k^2}\int_0^R \sin^2 kr dr = C^2\frac{1}{k^2}\int_0^R \left(\frac{1}{2} - \frac{1}{2}\cos kr\right) dr = C^2\frac{1}{k^2}\left(\frac{R}{2}\right) \rightarrow C = \sqrt{\frac{2k^2}{R}}$$

Therefore,

$$\psi(r,\theta,\phi) = \sqrt{\frac{1}{2\pi R}}\frac{\sin kr}{r}$$

and the first-order energy correction is

$$E^{(1)} = \frac{e^2B^2}{8mc^2}\frac{1}{2\pi R}\int_0^R r^2\sin^2 kr\,dr\int_0^\pi 2\pi\sin^3\theta d\theta = \left(\frac{1}{3}-\frac{1}{2\pi^2}\right)\frac{e^2B^2R^2}{12mc^2}$$

where we have used

$$\sin kR = 0 \rightarrow kR = \pi$$

(c) Suppose that, instead a weak uniform electric field of strength $\mathcal{E}$ is switched on. Will the ground state energy increase or decrease? Write down, but do not attempt to evaluate, a formula for the shift in the ground state energy due to the electric field.

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

$$E_\varepsilon^{(2)} = \sum_{m\neq 0=ground\ state}\frac{|V_{m0}|^2}{E_0^{(0)}-E_m^{(0)}}$$

But, $E_0^{(0)} < E_m^{(0)}$ $(m \neq 0)$ 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

$$\hat{H} = \frac{\vec{p}^2}{2m} + \frac{e^2B^2}{8mc^2}\left(\hat{x}^2+\hat{y}^2\right)$$

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

$$\frac{1}{2}m\omega^2 = \frac{e^2B^2}{8mc^2} \rightarrow \omega = \frac{eB}{2mc}$$

8.9.23 Hydrogen in electric and magnetic fields

Consider the $n=2$ levels of a hydrogen-like atom. Neglect spins. Calculate to lowest order the energy splittings in the presence of both electric and magnetic fields $\vec{B}=B\hat{e}_z$ and $\vec{\mathcal{E}}=\mathcal{E}\hat{e}_x$.

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

$$\begin{aligned}\hat{V}&=V_{electric}+V_{magnetic}\\&=-\vec{\mu}\cdot\vec{\varepsilon}-\frac{e}{mc}\vec{p}\cdot\vec{A}=-e\vec{r}\cdot\vec{\varepsilon}-\frac{e}{mc}\vec{p}\cdot\vec{A}\\&=-e\vec{r}\cdot\varepsilon\hat{e}_x-\frac{e}{mc}\vec{p}\cdot\vec{A}=-e\varepsilon\hat{x}-\frac{e}{mc}\vec{p}\cdot\vec{A}\end{aligned}$$

Now, $\vec{B}=B\hat{e}_z$, which says that $\vec{A}=Br\hat{e}_\phi$ so that

$$-\frac{e}{mc}\vec{p}\cdot\vec{A}=-\frac{e}{mc}p_\phi Br=-\frac{eB}{mc}r\frac{\hbar}{i}\frac{\partial}{\partial\phi}=\frac{\hbar\omega_c}{i}\frac{\partial}{\partial\phi}=\omega_c\hat{L}_z\quad,\quad\omega_c=-\frac{eB}{mc}$$

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,

$$\langle L'M'|\,V_{magnetic}\,|LM\rangle=M\hbar\omega_c\delta_{L'L}\delta_{M'M}\rightarrow\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&\hbar\omega_c&0\\0&0&0&-\hbar\omega_c\end{pmatrix}$$

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.

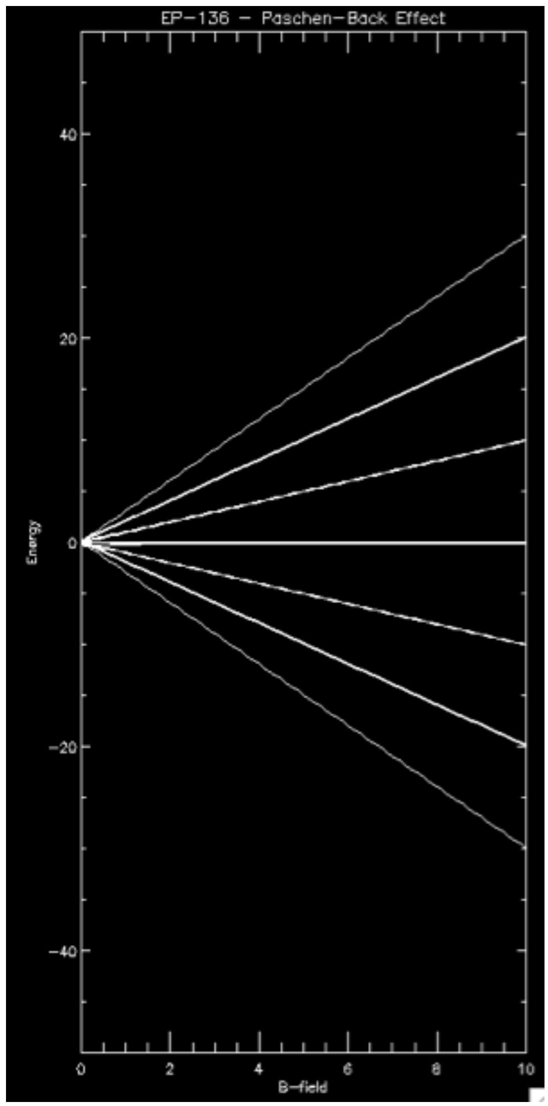
$$\langle 0,0|\,\hat{x}\,|1,0\rangle\propto\frac{1}{2}\int_0^{2\pi}\left(e^{i\phi}+e^{-i\phi}\right)d\phi=0$$

Therefore, the full$V$ matrix in the degenerate subspace is

$$\begin{pmatrix}0&0&0&0\\0&0&\varsigma&\varsigma\\0&\varsigma&\hbar\omega_c&0\\0&\varsigma&0&-\hbar\omega_c\end{pmatrix}$$

The eigenvalues are

$$
\begin{array}{llll}
 & - - - - - - - - - - - - - - - & E_2^{(0)} + \Delta & \text{non - degenerate} \\
E_2^{(0)} - - - - - - - - - - - - - & - - - - - - - - - - - - - - - & E_2^{(0)} & \text{2 - fold degenerate} \\
 & - - - - - - - - - - - - - - - & E_2^{(0)} - \Delta & \text{non - degenerate}
\end{array}
$$



8.9.24 $n = 3$ 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

$$V = e\varepsilon r\cos\theta$$

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

$$\begin{aligned}&\ell = 2\ ,\ m = \pm 2, \pm 1, 0 \to 5\ states\\ &\ell = 1\ ,\ m = \pm 1, 0 \to 3\ states\\ &\ell = 0\ ,\ m = 0 \to 1\ state\end{aligned}$$

We denote the zero-order state vectors as $|\ell, m\rangle$

$$\begin{array}{lllll} |1\rangle = |2,2\rangle & , & |2\rangle = |2,-2\rangle & , & |3\rangle = |2,1\rangle \\ |4\rangle = |1,1\rangle & , & |5\rangle = |2,-1\rangle & , & |6\rangle = |1,-1\rangle \\ |7\rangle = |2,0\rangle & , & |8\rangle = |1,0\rangle & , & |9\rangle = |0,0\rangle \end{array}$$

The degenerate submatrix is $9 \times 9 = 81$ elements. Because it is Hermitian, there are 45 independent elements to determine.

Now $\cos\theta \propto Y_{10}$ so that each matrix element contains the factor

$$\langle \ell m| Y_{10} |\ell' m'\rangle = 0 \quad unless \quad m = m' \ and\ \ell' = \ell + 1$$

These relations are called *selection rules* (More about selection rules in Chapter 11). They say that the only nonzero matrix elements of V are

$$\begin{array}{lll} \langle 3| V |4\rangle = \langle 4| V |3\rangle = a & , & \langle 5| V |6\rangle = \langle 6| V |5\rangle = b \\ \langle 7| V |8\rangle = \langle 8| V |7\rangle = c & , & \langle 8| V |9\rangle = \langle 9| V |8\rangle = d \end{array}$$

We will evaluate the matrix elements later.

The matrix is

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & c & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & c & 0 & d \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & d & 0 \end{pmatrix}$$

We have two 2×2 and one 3×3 submatrices to diagonalize. The eigenvalues give the first-order energy corrections. We have

$$\begin{aligned}
E_1^{(1)} &= E_2^{(1)} = 0 \quad 1x1\ matrices \\
E_{3,4}^{(1)} &= \pm a \quad 2x2\ matrix \\
E_{5,6}^{(1)} &= \pm b \quad 2x2\ matrix \\
E_{7,8,9}^{(1)} &= 0, \pm\sqrt{c^2+d^2} \quad 3x3\ matrix
\end{aligned}$$

Calculation of matrix elements:

Radial/Angular functions:

$$\begin{aligned}
R_{32}(r) &= \tfrac{2\sqrt{2}}{27\sqrt{5}}\left(\tfrac{1}{3a_0}\right)^{3/2}\left(\tfrac{r}{a_0}\right)^2 e^{-r/3a_0} \\
R_{31}(r) &= \tfrac{4\sqrt{2}}{9}\left(\tfrac{1}{3a_0}\right)^{3/2}\left(\tfrac{r}{a_0}\right)\left(1-\tfrac{r}{6a_0}\right) e^{-r/3a_0} \\
R_{30}(r) &= 2\left(\tfrac{1}{3a_0}\right)^{3/2}\left(1-\tfrac{2r}{3a_0}+\tfrac{2r^2}{9a_0^2}\right) e^{-r/3a_0}
\end{aligned}$$

$$\begin{aligned}
Y_{2,\pm 2} &= \sqrt{\tfrac{15}{32\pi}}e^{\pm 2i\phi}\sin^2\theta \quad , \quad Y_{2,\pm 1} = -\sqrt{\tfrac{15}{8\pi}}e^{\pm i\phi}\sin\theta\cos\theta \\
Y_{2,0} &= \sqrt{\tfrac{5}{16\pi}}\left(3\cos^2\theta-1\right) \quad , \quad Y_{1,\pm 1} = -\sqrt{\tfrac{3}{8\pi}}e^{\pm i\phi}\sin\theta \\
Y_{1,0} &= \sqrt{\tfrac{3}{4\pi}}\cos\theta \quad , \quad Y_{0,0} = \sqrt{\tfrac{1}{4\pi}}
\end{aligned}$$

Now

$$\begin{aligned}
a &= \langle 4|V|3\rangle = \langle 11|V|21\rangle = e\varepsilon\int_0^\infty\int_0^{2\pi}\int_1^{-1} r^2 dr d\phi d(\cos\theta) r\cos\theta R_{31}R_{32}Y_{11}^*Y_{21} \\
&= e\varepsilon\frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{1}{3a_0}\right)^3\frac{4\sqrt{2}}{9}\sqrt{\frac{3}{8\pi}}\sqrt{\frac{15}{8\pi}} \\
&\quad\times\int_0^\infty r^3\left(\frac{r}{a_0}\right)^3\left(1-\frac{r}{6a_0}\right)e^{-2r/3a_0}dr\int_0^{2\pi}d\phi e^{-i\phi}e^{+i\phi}\int_1^{-1}d(\cos\theta)\sin^2\theta\cos^2\theta \\
&= e\varepsilon a_0\frac{2}{3^7\pi}\left(\int_0^\infty x^6\left(1-\frac{x}{6}\right)e^{-2x/3}dx\right)\left(\int_0^{2\pi}d\phi\right)\left(\int_1^{-1}dy(1-y^2)y^2\right) \\
&= e\varepsilon a_0\frac{2}{3^7\pi}(2\pi)\left(\int_0^\infty x^6 e^{-2x/3}dx-\frac{1}{6}\int_0^\infty x^7 e^{-2x/3}dx\right)\left(-\frac{4}{15}\right) \\
&= -e\varepsilon a_0\frac{16}{5\cdot 3^8}\left(\int_0^\infty x^6 e^{-2x/3}dx-\frac{1}{6}\int_0^\infty x^7 e^{-2x/3}dx\right) \\
&= -e\varepsilon a_0\frac{16}{5\cdot 3^8}\left(\frac{6!}{\left(\frac{2}{3}\right)^7}-\frac{1}{6}\frac{7!}{\left(\frac{2}{3}\right)^8}\right) = \frac{9}{2}e\varepsilon a_0
\end{aligned}$$

Similarly,

$$b = \frac{9}{2}e\varepsilon a_0 \quad , \quad c = 3\sqrt{3}e\varepsilon a_0 \quad , \quad d = 3\sqrt{6}e\varepsilon a_0$$

Therefore, the energy levels to first-order are

$$\begin{array}{l} E = -\frac{e^2}{18a_0} \quad (3-\text{fold degenerate}) \\ E = -\frac{e^2}{18a_0} + \frac{9}{2}e\varepsilon a_0 \quad (2-\text{fold degenerate}) \\ E = -\frac{e^2}{18a_0} - \frac{9}{2}e\varepsilon a_0 \quad (2-\text{fold degenerate}) \\ E = -\frac{e^2}{18a_0} + 9e\varepsilon a_0 \quad (\text{non}-\text{degenerate}) \\ E = -\frac{e^2}{18a_0} - 9e\varepsilon a_0 \quad (\text{non}-\text{degenerate}) \end{array}$$

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).

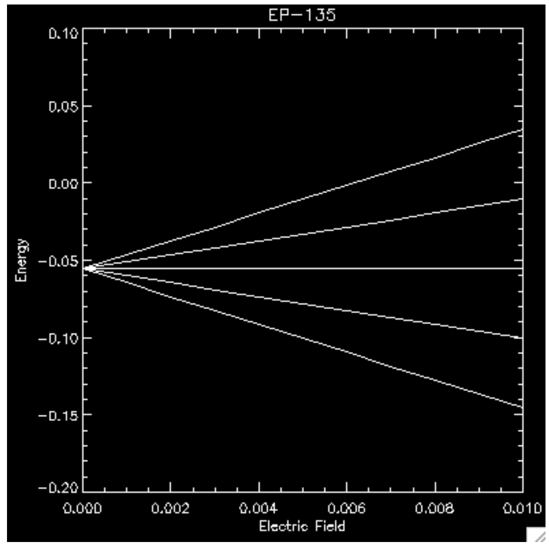
Zero-order state vectors:

$$\begin{array}{l} |\bar{1}\rangle = |1\rangle \quad , \quad E = -\frac{e^2}{18a_0} \\ |\bar{2}\rangle = |2\rangle \quad , \quad E = -\frac{e^2}{18a_0} \\ |\bar{3}\rangle = \frac{1}{\sqrt{2}}(|3\rangle + |4\rangle) \quad , \quad E = -\frac{e^2}{18a_0} - \frac{9}{2}e\varepsilon a_0 \\ |\bar{4}\rangle = \frac{1}{\sqrt{2}}(|3\rangle - |4\rangle) \quad , \quad E = -\frac{e^2}{18a_0} + \frac{9}{2}e\varepsilon a_0 \\ |\bar{5}\rangle = \frac{1}{\sqrt{2}}(|5\rangle + |6\rangle) \quad , \quad E = -\frac{e^2}{18a_0} - \frac{9}{2}e\varepsilon a_0 \\ |\bar{6}\rangle = \frac{1}{\sqrt{2}}(|5\rangle - |6\rangle) \quad , \quad E = -\frac{e^2}{18a_0} + \frac{9}{2}e\varepsilon a_0 \\ |\bar{7}\rangle = \sqrt{\frac{1}{6}}|7\rangle - \sqrt{\frac{1}{2}}|8\rangle + \sqrt{\frac{1}{3}}|9\rangle \quad , \quad E = -\frac{e^2}{18a_0} - 9e\varepsilon a_0 \\ |\bar{8}\rangle = -\sqrt{\frac{2}{3}}|7\rangle + \sqrt{\frac{1}{3}}|9\rangle \quad , \quad E = -\frac{e^2}{18a_0} \\ |\bar{9}\rangle = \sqrt{\frac{1}{6}}|7\rangle + \sqrt{\frac{1}{2}}|8\rangle + \sqrt{\frac{1}{3}}|9\rangle \quad , \quad E = -\frac{e^2}{18a_0} + 9e\varepsilon a_0 \end{array}$$

If we choose the values $e^2 = 1 = a_0$ so that

$$\begin{array}{l} E = -\frac{1}{18} \\ E = -\frac{1}{18} + \frac{9}{2}\varepsilon \\ E = -\frac{1}{18} - \frac{9}{2}\varepsilon \\ E = -\frac{1}{18} + 9\varepsilon \\ E = -\frac{1}{18} - 9\varepsilon \end{array}$$

we get a plot that looks like:



8.9.25 Perturbation of the $n = 3$ level in Hydrogen - Spin-Orbit and Magnetic Field corrections

In this problem we want to calculate the 1st-order correction to the n=3 unperturbed energy of the hydrogen atom due to spin-orbit interaction and magnetic field interaction for arbitrary strength of the magnetic field. We have $\hat{H} = \hat{H}_0 + \hat{H}_{so} + \hat{H}_m$ where

$$\hat{H}_0 = \frac{\vec{p}_{op}^2}{2m} + V(r) \quad , \quad V(r) = -e^2\left(\frac{1}{r}\right)$$
$$\hat{H}_{so} = \left[\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right]\vec{S}_{op}\cdot\vec{L}_{op}$$
$$\hat{H}_m = \frac{\mu_B}{\hbar}(\vec{L}_{op} + 2\vec{S}_{op})\cdot\vec{B}$$

We have two possible choices for basis functions, namely,

$$|n\ell s m_\ell m_s\rangle \quad or \quad |n\ell s j m_j\rangle$$

The former are easy to write down as direct-product states

$$|n\ell s m_\ell m_s\rangle = R_{n\ell}(r)Y_\ell^{m_\ell}(\theta,\varphi)\,|s,m_s\rangle$$

while the latter must be constructed from these direct-product states using addition of angular momentum methods. The perturbation matrix is not diagonal in either basis. The number of basis states is given by

$$\sum_{\ell=0}^{n-1=2}(2\ell+1)\times 2 = 10 + 6 + 2 = 18$$

All the 18 states are degenerate in zero-order. This means that we deal with an 18×18 matrix (mostly zeroes) in degenerate perturbation theory.

Using the direct-product states

(a) Calculate the nonzero matrix elements of the perturbation and arrange them in block-diagonal form.

We have

$$\begin{aligned} \hat{H}_0 &= \frac{\vec{p}_{op}^{\,2}}{2m} + V(r) \quad , \quad V(r) = -e^2\left(\frac{1}{r}\right) \\ \hat{H}_{so} &= \left[\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right]\vec{S}_{op}\cdot\vec{L}_{op} \\ \hat{H}_m &= \frac{\mu_B}{\hbar}(\vec{L}_{op} + 2\vec{S}_{op})\cdot\vec{B} \end{aligned}$$

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

$$\begin{aligned} &\ell = 2\ ,\ m = \pm 2, \pm 1, 0 \to 5\ states \\ &\ell = 1\ ,\ m = \pm 1, 0 \to 3\ states \\ &\ell = 0\ ,\ m = 0 \to 1\ state \\ &s = 1/2\ ,\ m_s = \pm 1/2 \to 2\ states\ for\ each\ \ell\ state \end{aligned}$$

We denote the zero-order state vectors as $|\ell, m, m_s\rangle$.

$$\begin{aligned} &|1\rangle = |0,0,+\rangle\ ,\ |2\rangle = |0,0,-\rangle\ ,\ |3\rangle = |1,1,+\rangle\ ,\ |4\rangle = |1,1,-\rangle \\ &|5\rangle = |1,0,+\rangle\ ,\ |6\rangle = |1,0,-\rangle\ ,|7\rangle = |1,-1,+\rangle\ ,\ |8\rangle = |1,-1,-\rangle \\ &|9\rangle = |2,2,+\rangle\ ,\ |10\rangle = |2,2,-\rangle\ ,\ |11\rangle = |2,1,+\rangle\ ,\ |12\rangle = |2,1,-\rangle \\ &|13\rangle = |2,0,+\rangle\ ,\ |14\rangle = |2,0,-\rangle\ ,\ |15\rangle = |2,-1,+\rangle\ ,\ |16\rangle = |2,-1,-\rangle \\ &|17\rangle = |2,-2,+\rangle\ ,\ |18\rangle = |2,-2,-\rangle \end{aligned}$$

The degenerate matrix is $18 \times 18 = 324$ elements. Because it is Hermitian, there are 171 independent elements to determine.

The magnetic term

$$\hat{H}_m = \mu_B(\vec{L}_{op} + 2\vec{S}_{op})\cdot\vec{B}/\hbar$$

is diagonal in this basis as shown below:

$$\begin{aligned} \langle \ell', m', m_s'|\, \hat{H}_m\, |\ell, m, m_s\rangle &= \mu_B B\, \langle \ell', m', m_s'|\, (\hat{L}_z + 2\hat{S}_z\, |\ell, m, m_s\rangle \\ &= \mu_B B(m + 2m_s)\delta_{\ell'\ell}\delta_{m'm}\delta_{m_s' m_s} \end{aligned}$$

so we get the matrix

$$
\mu_B B \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3
\end{pmatrix}
$$

The spin-orbit term

$$\hat{H}_{so} = \left[\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right]\vec{S}_{op}\cdot\vec{L}_{op}$$

can be rewritten as

$$\hat{H}_{so} = \left[\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right]\vec{S}_{op}\cdot\vec{L}_{op} = \left[\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right]\left(\hat{L}_z\hat{S}_z + \frac{1}{2}\left(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+\right)\right)$$

This means that the matrix element

$$\begin{aligned}
&\langle \ell', m', m_s'|\,\hat{H}_{so}\,|\ell, m, m_s\rangle \\
&\quad = \langle \ell', m', m_s'|\left[\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right]\left(\hat{L}_z\hat{S}_z + \frac{1}{2}\left(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+\right)\right)|\ell, m, m_s\rangle
\end{aligned}$$

equals zero unless one of the following conditions holds:

$$\begin{aligned}
&(m' = m \;\&\; m_s' = m_s) \\
&or \\
&(m' + 1 = m \;\&\; m_s' - 1 = m_s) \\
&or \\
&(m' - 1 = m \;\&\; m_s' + 1 = m_s)
\end{aligned}$$

Therefore, we have to calculate all of the diagonal elements, but only the off-diagonal elements below:

$$\begin{aligned}
&\langle 4|\,\hat{H}_{so}\,|5\rangle \;,\; \langle 6|\,\hat{H}_{so}\,|7\rangle \;,\; \langle 10|\,\hat{H}_{so}\,|11\rangle \\
&\langle 12|\,\hat{H}_{so}\,|13\rangle \;,\; \langle 14|\,\hat{H}_{so}\,|15\rangle \;,\; \langle 16|\,\hat{H}_{so}\,|17\rangle
\end{aligned}$$

We also note that any diagonal element is zero if $m = 0$ and the matrix element is zero id $\ell = 0$.

Finally, we note that

$$\left\langle \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right\rangle_{n\ell} = \frac{e^2}{2m^2c^2}\langle n\ell|\frac{1}{r^3}|n\ell\rangle = \frac{e^2}{2m^2c^2}\left[\frac{Z^3}{a_0^3n^3\ell(\ell+1/2)(\ell+1)}\right]$$
$$= A\left[\frac{1}{\ell(\ell+1/2)(\ell+1)}\right]$$

where

$$A = \frac{Z^3e^2}{2m^2c^2a_0^3n^3} = \frac{e^2}{54m^2c^2a_0^3}$$

Therefore, we have

$$\left\langle \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right\rangle_{32} = \frac{A}{15} \quad , \quad \left\langle \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right\rangle_{31} = \frac{A}{3}$$

So let us do it.....

$$\langle 1|\hat{H}_{so}|1\rangle = \langle 2|\hat{H}_{so}|2\rangle = \langle 5|\hat{H}_{so}|5\rangle = 0$$
$$\langle 6|\hat{H}_{so}|6\rangle = \langle 13|\hat{H}_{so}|13\rangle = \langle 14|\hat{H}_{so}|14\rangle = 0$$

$$\langle 3|\hat{H}_{so}|3\rangle = \tfrac{A}{3}\langle 1,1,+|\hat{L}_z\hat{S}_z|1,1,+\rangle = \tfrac{A}{3}\left(\tfrac{\hbar^2}{2}\right) = \tfrac{A\hbar^2}{6}$$
$$\langle 4|\hat{H}_{so}|4\rangle = \tfrac{A}{3}\langle 1,1,-|\hat{L}_z\hat{S}_z|1,1,-\rangle = \tfrac{A}{3}\left(-\tfrac{\hbar^2}{2}\right) = -\tfrac{A\hbar^2}{6}$$
$$\langle 4|\hat{H}_{so}|5\rangle = \tfrac{A}{6}\langle 1,1,-|\hat{L}_+\hat{S}_-|1,0,+\rangle = \tfrac{A}{6}\left(\sqrt{2}\hbar^2\right) = \tfrac{\sqrt{2}A\hbar^2}{6}$$
$$\langle 6|\hat{H}_{so}|7\rangle = \tfrac{A}{6}\langle 1,0,-|\hat{L}_+\hat{S}_-|1,-1,+\rangle = \tfrac{A}{6}\left(\sqrt{2}\hbar^2\right) = \tfrac{\sqrt{2}A\hbar^2}{6}$$
$$\langle 7|\hat{H}_{so}|7\rangle = \tfrac{A}{3}\langle 1,-1,+|\hat{L}_z\hat{S}_z|1,-1,+\rangle = \tfrac{A}{3}\left(-\tfrac{\hbar^2}{2}\right) = -\tfrac{A\hbar^2}{6}$$
$$\langle 8|\hat{H}_{so}|8\rangle = \tfrac{A}{3}\langle 1,-1,-|\hat{L}_z\hat{S}_z|1,-1,-\rangle = \tfrac{A}{3}\left(\tfrac{\hbar^2}{2}\right) = \tfrac{A\hbar^2}{6}$$
$$\langle 9|\hat{H}_{so}|9\rangle = \tfrac{A}{15}\langle 2,2,-|\hat{L}_z\hat{S}_z|2,2,+\rangle = \tfrac{A}{15}\left(\hbar^2\right) = \tfrac{A\hbar^2}{15}$$
$$\langle 10|\hat{H}_{so}|10\rangle = \tfrac{A}{15}\langle 2,2,-|\hat{L}_z\hat{S}_z|2,2,-\rangle = \tfrac{A}{15}\left(-\hbar^2\right) = -\tfrac{A\hbar^2}{15}$$
$$\langle 10|\hat{H}_{so}|11\rangle = \tfrac{A}{30}\langle 2,2,-|\hat{L}_+\hat{S}_-|2,1,+\rangle = \tfrac{A}{30}\left(2\hbar^2\right) = \tfrac{A\hbar^2}{15}$$
$$\langle 11|\hat{H}_{so}|11\rangle = \tfrac{A}{15}\langle 2,1,+|\hat{L}_z\hat{S}_z|2,1,+\rangle = \tfrac{A}{30}\left(\hbar^2\right) = \tfrac{A\hbar^2}{30}$$
$$\langle 12|\hat{H}_{so}|12\rangle = \frac{A}{15}\langle 2,1,-|\hat{L}_z\hat{S}_z|2,1,-\rangle = \frac{A}{30}\left(-\hbar^2\right) = -\frac{A\hbar^2}{30}$$
$$\langle 12|\hat{H}_{so}|13\rangle = \frac{A}{30}\langle 2,1,-|\hat{L}_+\hat{S}_-|2,0,+\rangle = \frac{A}{30}\left(\sqrt{6}\hbar^2\right) = \frac{\sqrt{6}A\hbar^2}{30}$$
$$\langle 14|\hat{H}_{so}|15\rangle = \tfrac{A}{30}\langle 2,0,-|\hat{L}_+\hat{S}_-|2,-1,+\rangle = \tfrac{A}{30}\left(\sqrt{6}\hbar^2\right) = \tfrac{\sqrt{6}A\hbar^2}{30}$$
$$\langle 15|\hat{H}_{so}|15\rangle = \tfrac{A}{15}\langle 2,-1,+|\hat{L}_z\hat{S}_z|2,-1,+\rangle = \tfrac{A}{15}\left(-\tfrac{\hbar^2}{2}\right) = -\tfrac{A\hbar^2}{30}$$
$$\langle 16|\hat{H}_{so}|16\rangle = \tfrac{A}{15}\langle 2,-1,-|\hat{L}_z\hat{S}_z|2,-1,-\rangle = \tfrac{A}{15}\left(\tfrac{\hbar^2}{2}\right) = \tfrac{A\hbar^2}{30}$$
$$\langle 16|\hat{H}_{so}|17\rangle = \tfrac{A}{30}\langle 2,-1,-|\hat{L}_+\hat{S}_-|2,-2,+\rangle = \tfrac{A}{30}\left(2\hbar^2\right) = \tfrac{A\hbar^2}{15}$$
$$\langle 17|\hat{H}_{so}|17\rangle = \tfrac{A}{15}\langle 2,-2,+|\hat{L}_z\hat{S}_z|2,-2,+\rangle = \tfrac{A}{15}\left(-\hbar^2\right) = -\tfrac{A\hbar^2}{15}$$
$$\langle 18|\hat{H}_{so}|18\rangle = \tfrac{A}{15}\langle 2,-2,-|\hat{L}_z\hat{S}_z|2,-2,-\rangle = \tfrac{A}{15}\left(\hbar^2\right) = \tfrac{A\hbar^2}{15}$$

Therefore, the corresponding matrix is as below:

$$\frac{A\hbar^2}{30}\begin{pmatrix}
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&5&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&-5&5\sqrt{2}&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&5\sqrt{2}&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&5\sqrt{2}&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&5\sqrt{2}&-5&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&5&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&-2&2&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&2&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&-1&\sqrt{6}&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&\sqrt{6}&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&\sqrt{6}&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&\sqrt{6}&-1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&2&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&-2&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2
\end{pmatrix}$$

(b) Diagonalize the blocks and determine the eigenvalues as functions of B.

We can read off the energies that are diagonal

$$\begin{aligned}
|1\rangle &\to E^{(1)} = \mu_B B \\
|2\rangle &\to E^{(1)} = -\mu_B B \\
|3\rangle &\to E^{(1)} = \tfrac{A\hbar^2}{6} + 2\mu_B B \\
|8\rangle &\to E^{(1)} = \tfrac{A\hbar^2}{6} - 2\mu_B B \\
|9\rangle &\to E^{(1)} = \tfrac{A\hbar^2}{15} + 3\mu_B B \\
|18\rangle &\to E^{(1)} = \tfrac{A\hbar^2}{15} - 3\mu_B B
\end{aligned}$$

We then need to diagonalize these remaining six 2×2 submatrices.

$$4-5 \quad \begin{pmatrix} -5\frac{A\hbar^2}{30} & 5\sqrt{2}\frac{A\hbar^2}{30} \\ 5\sqrt{2}\frac{A\hbar^2}{30} & \mu_B B \end{pmatrix}$$

$$6-7 \quad \begin{pmatrix} -\mu_B B & 5\sqrt{2}\frac{A\hbar^2}{30} \\ 5\sqrt{2}\frac{A\hbar^2}{30} & -5\frac{A\hbar^2}{30} \end{pmatrix}$$

$$10-11 \quad \begin{pmatrix} -2\frac{A\hbar^2}{30} + \mu_B B & 2\frac{A\hbar^2}{30} \\ 2\frac{A\hbar^2}{30} & \frac{A\hbar^2}{30} + 2\mu_B B \end{pmatrix}$$

$$12-13 \quad \begin{pmatrix} -\frac{A\hbar^2}{30} & \sqrt{6}\frac{A\hbar^2}{30} \\ \sqrt{6}\frac{A\hbar^2}{30} & \mu_B B \end{pmatrix}$$

$$14-15 \quad \begin{pmatrix} -\mu_B B & \sqrt{6}\frac{A\hbar^2}{30} \\ \sqrt{6}\frac{A\hbar^2}{30} & -\frac{A\hbar^2}{30} \end{pmatrix}$$

$$16-17 \quad \begin{pmatrix} \frac{A\hbar^2}{30} - 2\mu_B B & 2\frac{A\hbar^2}{30} \\ 2\frac{A\hbar^2}{30} & -2\frac{A\hbar^2}{30} - \mu_B B \end{pmatrix}$$

We get characteristic equations:

$$4-5 \quad \begin{pmatrix} -5\frac{A\hbar^2}{30} & 5\sqrt{2}\frac{A\hbar^2}{30} \\ 5\sqrt{2}\frac{A\hbar^2}{30} & \mu_B B \end{pmatrix} \rightarrow (E-\mu_B B)(E+\frac{A\hbar^2}{6}) - \frac{1}{18}\left(A\hbar^2\right)^2 = 0$$

$$6-7 \quad \begin{pmatrix} -\mu_B B & 5\sqrt{2}\frac{A\hbar^2}{30} \\ 5\sqrt{2}\frac{A\hbar^2}{30} & -5\frac{A\hbar^2}{30} \end{pmatrix} \rightarrow (E+\mu_B B)(E+\frac{A\hbar^2}{6}) - \frac{1}{18}\left(A\hbar^2\right)^2 = 0$$

$$10-11 \quad \begin{pmatrix} -2\frac{A\hbar^2}{30} + \mu_B B & 2\frac{A\hbar^2}{30} \\ 2\frac{A\hbar^2}{30} & \frac{A\hbar^2}{30} + 2\mu_B B \end{pmatrix} \rightarrow (E-\mu_B B+\frac{A\hbar^2}{15})(E-\frac{A\hbar^2}{30}-2\mu_B B) - \left(\frac{A\hbar^2}{15}\right)^2 = 0$$

$$12-13 \quad \begin{pmatrix} -\frac{A\hbar^2}{30} & \sqrt{6}\frac{A\hbar^2}{30} \\ \sqrt{6}\frac{A\hbar^2}{30} & \mu_B B \end{pmatrix} \rightarrow (E-\mu_B B)(E+\frac{A\hbar^2}{30}) - \frac{1}{150}\left(A\hbar^2\right)^2 = 0$$

$$14-15 \quad \begin{pmatrix} -\mu_B B & \sqrt{6}\frac{A\hbar^2}{30} \\ \sqrt{6}\frac{A\hbar^2}{30} & -\frac{A\hbar^2}{30} \end{pmatrix} \rightarrow (E+\mu_B B)(E+\frac{A\hbar^2}{30}) - \frac{1}{150}\left(A\hbar^2\right)^2 = 0$$

$$16-17 \quad \begin{pmatrix} \frac{A\hbar^2}{30} - 2\mu_B B & 2\frac{A\hbar^2}{30} \\ 2\frac{A\hbar^2}{30} & -2\frac{A\hbar^2}{30} - \mu_B B \end{pmatrix} \rightarrow (E+\mu_B B+\frac{A\hbar^2}{15})(E+2\mu_B B-\frac{A\hbar^2}{30}) - \left(\frac{A\hbar^2}{15}\right)^2 = 0$$

Continuing 4-5

$$\begin{aligned} E &= \frac{1}{2}\left(\mu_B B - \frac{A\hbar^2}{6}\right) \pm \frac{1}{2}\sqrt{\left(\mu_B B - \frac{A\hbar^2}{6}\right)^2 + \frac{2}{9}\left(A\hbar^2\right)^2 + \mu_B B\frac{2A\hbar^2}{3}} \\ &= \frac{1}{2}\left(\mu_B B - \frac{A\hbar^2}{6}\right) \pm \frac{1}{2}\sqrt{\frac{1}{4}\left(A\hbar^2\right)^2 + \frac{1}{3}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \end{aligned}$$

6-7

$$\begin{aligned} E &= -\frac{1}{2}\left(\frac{A\hbar^2}{6} + \mu_B B\right) \pm \frac{1}{2}\sqrt{\left(\frac{A\hbar^2}{6} + \mu_B B\right)^2 + \frac{2}{9}\left(A\hbar^2\right)^2 - \mu_B B\frac{2A\hbar^2}{3}} \\ &= -\frac{1}{2}\left(\frac{A\hbar^2}{6} + \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{4}\left(A\hbar^2\right)^2 - \frac{1}{3}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \end{aligned}$$

10-11

$$\begin{aligned} E &= -\frac{1}{2}\left(\frac{A\hbar^2}{30} - 3\mu_B B\right) \pm \sqrt{\left(\frac{A\hbar^2}{30} - 3\mu_B B\right)^2 + 4\left(\frac{A\hbar^2}{15}\right)^2 + 4\left(\frac{A\hbar^2}{30} + 2\mu_B B\right)\left(\frac{A\hbar^2}{15} - \mu_B B\right)} \\ &= -\frac{1}{2}\left(\frac{A\hbar^2}{30} - 3\mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 + \frac{1}{5}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \end{aligned}$$

12-13

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} - \mu_B B\right) \pm \frac{1}{2}\sqrt{\left(\frac{A\hbar^2}{30} - \mu_B B\right)^2 + 4\frac{1}{150}\left(A\hbar^2\right)^2 + 4\mu_B B\frac{A\hbar^2}{30}}$$
$$= -\frac{1}{2}\left(\frac{A\hbar^2}{30} - \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 + \frac{1}{15}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$

14-15

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} + \mu_B B\right) \pm \frac{1}{2}\sqrt{\left(\frac{A\hbar^2}{30} + \mu_B B\right)^2 + 4\frac{1}{150}\left(A\hbar^2\right)^2 - 4\mu_B B\frac{A\hbar^2}{30}}$$
$$= -\frac{1}{2}\left(\frac{A\hbar^2}{30} + \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 - \frac{1}{15}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$

16-17

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} + 3\mu_B B\right)$$
$$\pm \frac{1}{2}\sqrt{\left(\frac{A\hbar^2}{30} + 3\mu_B B\right)^2 + 4\left(\frac{A\hbar^2}{15}\right)^2 + 4\left(\frac{A\hbar^2}{15} + \mu_B B\right)\left(\frac{A\hbar^2}{30} - 2\mu_B B\right)}$$
$$= -\frac{1}{2}\left(\frac{A\hbar^2}{30} + 3\mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 - \frac{1}{5}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$

(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

$$E = \frac{1}{2}\left(\mu_B B - \frac{A\hbar^2}{6}\right) \pm \frac{1}{2}\sqrt{\frac{1}{4}\left(A\hbar^2\right)^2 + \frac{1}{3}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$
$$\to \frac{1}{6}A\hbar^2 + \frac{2}{3}\mu_B B \;\;,\;\; -\frac{1}{3}A\hbar^2 + \frac{1}{3}\mu_B B$$

6-7

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{6} + \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{4}\left(A\hbar^2\right)^2 - \frac{1}{3}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$
$$\to \frac{1}{6}A\hbar^2 - \frac{2}{3}\mu_B B \;\;,\;\; -\frac{1}{3}A\hbar^2 - \frac{1}{3}\mu_B B$$

10-11

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} - 3\mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 + \frac{1}{5}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$
$$\to \frac{1}{15}A\hbar^2 + \frac{9}{5}\mu_B B \;\;,\;\; -\frac{1}{10}A\hbar^2 + \frac{6}{5}\mu_B B$$

12-13

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} - \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 + \frac{1}{15}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$
$$\to \frac{1}{15}A\hbar^2 + \frac{3}{5}\mu_B B \;\;,\;\; -\frac{1}{10}A\hbar^2 + \frac{2}{5}\mu_B B$$

14-15

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} + \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 - \frac{1}{15}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$
$$\to \frac{1}{15}A\hbar^2 - \frac{3}{5}\mu_B B \;\;,\;\; -\frac{1}{10}A\hbar^2 - \frac{2}{5}\mu_B B$$

16-17

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} + 3\mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 - \frac{1}{5}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2}$$
$$\to \frac{1}{15}A\hbar^2 - \frac{9}{5}\mu_B B \;\;,\;\; -\frac{1}{10}A\hbar^2 - \frac{6}{5}\mu_B B$$

Spin-Orbit Levels

These levels go like

$$\frac{A\hbar^2}{2}\frac{(j(j+1) - \ell(\ell+1) - s(s+1))}{\ell(\ell+1/2)(\ell+1)}$$

so that

$$0 \to |1\rangle\,,|2\rangle \to \ell = 0\;,\; s = 1/2\;,\; j = 1/2$$
$$+\tfrac{A\hbar^2}{6} \to |3\rangle\,,|8\rangle\,,|\bar{4}\rangle\,,|\bar{6}\rangle \to \ell = 1\;,\; s = 1/2\;,\; j = 3/2$$
$$+\tfrac{A\hbar^2}{15} \to |9\rangle\,,|18\rangle\,,\left|\overline{10}\right\rangle,\left|\overline{12}\right\rangle,\left|\overline{14}\right\rangle,\left|\overline{16}\right\rangle \to \ell = 2\;,\; s = 1/2\;,\; j = 5/2$$
$$-\tfrac{A\hbar^2}{3} \to \left|\overline{5}\right\rangle,\left|\overline{7}\right\rangle \to \ell = 1\;,\; s = 1/2\;,\; j = 1/2$$
$$-\tfrac{A\hbar^2}{10} \to \left|\overline{11}\right\rangle,\left|\overline{13}\right\rangle,\left|\overline{15}\right\rangle,\left|\overline{17}\right\rangle \to \ell = 2\;,\; s = 1/2\;,\; j = 3/2$$

in agreement with the spin-orbit formula.

(d) Look at the large B limit. Identify the Paschen-Bach levels.

The $B \to \infty$ limit:

$$|1\rangle \to +\mu_B B$$
$$|2\rangle \to -\mu_B B$$
$$|3\rangle \to +2\mu_B B$$
$$|8\rangle \to -2\mu_B B$$
$$|9\rangle \to +3\mu_B B$$
$$|18\rangle \to -3\mu_B B$$

4-5

$$E = \frac{1}{2}\left(\mu_B B - \frac{A\hbar^2}{6}\right) \pm \frac{1}{2}\sqrt{\frac{1}{4}\left(A\hbar^2\right)^2 + \frac{1}{3}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \to \mu_B B \;\;,\;\; 0$$

6-7

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{6} + \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{4}\left(A\hbar^2\right)^2 - \frac{1}{3}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \to 0 \;\;,\;\; -\mu_B B$$

10-11

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} - 3\mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 + \frac{1}{5}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \to 2\mu_B B \;\;,\;\; \mu_B B$$

12-13

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} - \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 + \frac{1}{15}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \to \mu_B B \ \ , \ \ 0$$

14-15

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} + \mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 - \frac{1}{15}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \to 0 \ \ , \ \ -\mu_B B$$

16-17

$$E = -\frac{1}{2}\left(\frac{A\hbar^2}{30} + 3\mu_B B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36}\left(A\hbar^2\right)^2 - \frac{1}{5}\mu_B B A\hbar^2 + \left(\mu_B B\right)^2} \to -\mu_B B \ \ , \ \ -2\mu_B B$$

The Paschen-Back levels are

$$\begin{aligned}
&3\mu_B B \to |9\rangle \\
&2\mu_B B \to |3\rangle , \left|\overline{10}\right\rangle \\
&\mu_B B \to |1\rangle , \left|\bar{4}\right\rangle , \left|\overline{11}\right\rangle , \left|\overline{12}\right\rangle \\
&0 \to \left|\bar{5}\right\rangle , \left|\bar{6}\right\rangle , \left|\overline{13}\right\rangle , \left|\overline{14}\right\rangle \\
&-\mu_B B \to |2\rangle , \left|\bar{7}\right\rangle , \left|\overline{15}\right\rangle , \left|\overline{16}\right\rangle \\
&-2\mu_B B \to |8\rangle , \left|\overline{17}\right\rangle \\
&-3\mu_B B \to |18\rangle
\end{aligned}$$

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

$$\begin{aligned}
&|1\rangle , |2\rangle \to \ell = 0 \ , \ s = 1/2 \ , \ j = 1/2 \\
&|3\rangle , |8\rangle , |\bar{4}\rangle , |\bar{6}\rangle \to \ell = 1 \ , \ s = 1/2 \ , \ j = 3/2 \\
&|9\rangle , |18\rangle , \left|\overline{10}\right\rangle , \left|\overline{12}\right\rangle , \left|\overline{14}\right\rangle , \left|\overline{16}\right\rangle \to \ell = 2 \ , \ s = 1/2 \ , \ j = 5/2 \\
&\left|\bar{5}\right\rangle , \left|\bar{7}\right\rangle \to \ell = 1 \ , \ s = 1/2 \ , \ j = 1/2 \\
&\left|\overline{11}\right\rangle , \left|\overline{13}\right\rangle , \left|\overline{15}\right\rangle , \left|\overline{17}\right\rangle \to \ell = 2 \ , \ s = 1/2 \ , \ j = 3/2
\end{aligned}$$

The Lande-g factor is

$$g = 1 + \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)}$$

The levels go like: $E_{so} + g m_j \mu_B B$

$$\begin{aligned}
&|1\rangle , |2\rangle \to \ell = 0 \ , \ s = 1/2 \ , \ j = 1/2 \to g = 2 \\
&|3\rangle , |8\rangle , |\bar{4}\rangle , |\bar{6}\rangle \to \ell = 1 \ , \ s = 1/2 \ , \ j = 3/2 \to g = 4/3 \\
&|9\rangle , |18\rangle , \left|\overline{10}\right\rangle , \left|\overline{12}\right\rangle , \left|\overline{14}\right\rangle , \left|\overline{16}\right\rangle \to \ell = 2 \ , \ s = 1/2 \ , \ j = 5/2 \to g = 6/5 \\
&\left|\bar{5}\right\rangle , \left|\bar{7}\right\rangle \to \ell = 1 \ , \ s = 1/2 \ , \ j = 1/2 \to g = 2/3 \\
&\left|\overline{11}\right\rangle , \left|\overline{13}\right\rangle , \left|\overline{15}\right\rangle , \left|\overline{17}\right\rangle \to \ell = 2 \ , \ s = 1/2 \ , \ j = 3/2 \to g = 4/5
\end{aligned}$$

$$
\begin{aligned}
&|1\rangle \to \mu_B B \to g m_j = (2)\,(1/2)\\
&|2\rangle \to -\mu_B B \to g m_j = (2)\,(-1/2)\\
&|3\rangle \to \tfrac{A\hbar^2}{6} + 2\mu_B B \to g m_j = (4/3)\,(3/2)\\
&|8\rangle \to \tfrac{A\hbar^2}{6} - 2\mu_B Bb \to g m_j = (4/3)\,(-3/2)\\
&|9\rangle \to \tfrac{A\hbar^2}{15} + 3\mu_B B \to g m_j = (6/5)\,(5/2)\\
&|18\rangle \to \tfrac{A\hbar^2}{15} - 3\mu_B B \to g m_j = (6/5)\,(-5/2)
\end{aligned}
$$

4-5

$$\frac{1}{6}A\hbar^2 + \frac{2}{3}\mu_B B \;\;,\;\; -\frac{1}{3}A\hbar^2 + \frac{1}{3}\mu_B B \to g m_j = (4/3)\,(1/2) \;\;,\;\; (2/3)\,(1/2)$$

6-7

$$\frac{1}{6}A\hbar^2 - \frac{2}{3}\mu_B B \;\;,\;\; -\frac{1}{3}\;A\hbar^2 - \frac{1}{3}\mu_B B \to g m_j = (4/3)\,(-1/2) \;\;,\;\; (2/3)\,(-1/2)$$

10-11

$$\frac{1}{15}A\hbar^2 + \frac{9}{5}\mu_B B \;\;,\;\; -\frac{1}{10}A\hbar^2 + \frac{6}{5}\mu_B B \to g m_j = (6/5)\,(3/2) \;\;,\;\; (4/5)\,(3/2)$$

12-13

$$\frac{1}{15}A\hbar^2 + \frac{3}{5}\mu_B B \;\;,\;\; -\frac{1}{10}A\hbar^2 + \frac{2}{5}\mu_B B \to g m_j = (6/5)\,(1/2) \;\;,\;\; (4/5)\,(1/2)$$

14-15

$$\frac{1}{15}A\hbar^2 - \frac{3}{5}\mu_B B \;\;,\;\; -\frac{1}{10}A\hbar^2 - \frac{2}{5}\mu_B B \to g m_j = (6/5)\,(-1/2)\;,\; (4/5)\,(-1/2)$$

16-17

$$\frac{1}{15}A\hbar^2 - \frac{9}{5}\mu_B B \;\;,\;\; -\frac{1}{10}A\hbar^2 - \frac{6}{5}\mu_B B \to g m_j = (6/5)\,(-3/2)\;,\; (4/5)\,(-3/2)$$

so that the results are in agreement with the Lande-g factor formula.

(f) Plot the eigenvalues versus B. We choose $\mu_B = 1 = A\hbar^2$ so that the energy levels become

$$
\begin{aligned}
&|1\rangle \to E = B\\
&|2\rangle \to E = -B\\
&|3\rangle \to E = \tfrac{1}{6} + 2B\\
&|8\rangle \to E = \tfrac{1}{6} - 2B\\
&|9\rangle \to E = \tfrac{1}{15} + 3B\\
&|18\rangle \to E = \tfrac{1}{15} - 3B
\end{aligned}
$$

4-5

$$E = \frac{1}{2}\left(B - \frac{1}{6}\right) \pm \frac{1}{2}\sqrt{\frac{1}{4} + \frac{1}{3}B + B^2}$$

6-7

$$E = -\frac{1}{2}\left(\frac{1}{6} + B\right) \pm \frac{1}{2}\sqrt{\frac{1}{4} - \frac{1}{3}B + B^2}$$

10-11

$$E = -\frac{1}{2}\left(\frac{1}{30} - 3B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36} + \frac{1}{5}B + B^2}$$

12-13

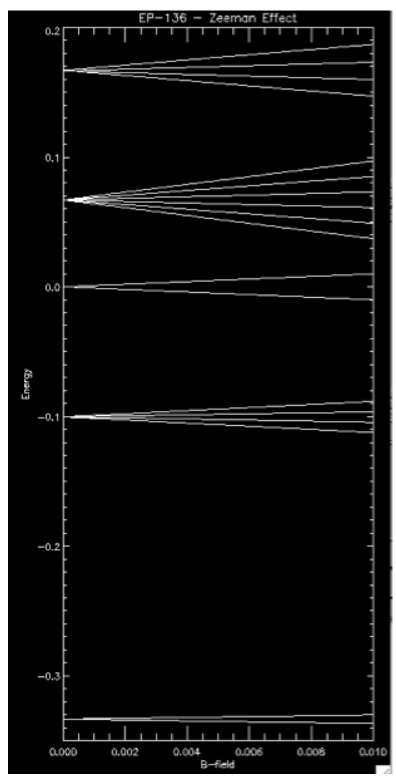
$$E = -\frac{1}{2}\left(\frac{1}{30} - B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36} + \frac{1}{15}B + B^2}$$

14-15

$$E = -\frac{1}{2}\left(\frac{1}{30} + B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36} - \frac{1}{15}B + B^2}$$

16-17

$$E = -\frac{1}{2}\left(\frac{1}{30} + 3B\right) \pm \frac{1}{2}\sqrt{\frac{1}{36} - \frac{1}{5}B + B^2}$$



8.9.26 Stark Shift in Hydrogen with Fine Structure

Excluding nuclear spin, the $n = 2$ spectrum of Hydrogen has the configuration:

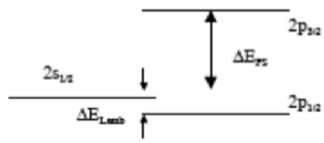


Figure 8.5: $n = 2$ Spectrum in Hydrogen

where $\Delta E_{FS}/\hbar = 10\ GHz$ (the fine structure splitting) and $\Delta E_{Lamb}/\hbar = 1\ GHz$ (the Lamb shift - an effect of quantum fluctuations of the electromagnetic field). These shifts were neglected in the text discussion of the Stark effect. This is valid if $ea_0E_z >> \Delta E$. Let $x = ea_0E_z$.

The diagram above shows the $n = 2$ energy levels in Hydrogen including fine structure. We now want to add a Stark effect perturbation $\hat{H}_{int} = +e\hat{z}E_z$ (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:

$$
\begin{aligned}
2s_{1/2} &\Rightarrow \left|2s_{1/2}, +1/2\right\rangle, \left|2s_{1/2}, -1/2\right\rangle \\
2p_{1/2} &\Rightarrow \left|2p_{1/2}, +1/2\right\rangle, \left|2p_{1/2}, -1/2\right\rangle \\
2p_{3/2} &\Rightarrow \left|2p_{3/2}, +3/2\right\rangle, \left|2p_{3/2}, +1/2\right\rangle, \left|2p_{3/2}, -1/2\right\rangle, \left|2p_{3/2}, -3/2\right\rangle
\end{aligned}
$$

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

$$
\begin{aligned}
\left|2s_{1/2}, \pm 1/2\right\rangle &= \left|2s, m_\ell = 0\right\rangle \otimes \left|m_s = \pm 1/2\right\rangle \\
\left|2p_{1/2}, \pm 1/2\right\rangle &= \sqrt{\tfrac{1}{3}} \left|2p, 0\right\rangle \otimes \left|\pm 1/2\right\rangle - \sqrt{\tfrac{2}{3}} \left|2p, \pm 1\right\rangle \otimes \left|\mp 1/2\right\rangle \\
\left|2p_{3/2}, \pm 1/2\right\rangle &= \sqrt{\tfrac{2}{3}} \left|2p, 0\right\rangle \otimes \left|\pm 1/2\right\rangle + \sqrt{\tfrac{1}{3}} \left|2p, \pm 1\right\rangle \otimes \left|\mp 1/2\right\rangle \\
\left|2p_{3/2}, \pm 3/2\right\rangle &= \left|2p, \pm 1\right\rangle \otimes \left|\pm 1/2\right\rangle
\end{aligned}
$$

(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 $ea_0E_z \leq \Delta E_{Lamb}$, we can restrict our attention to the

$(2s_{1/2}, 2p_{1/2})$ subspace.

The matrix representation of $\hat{H}_{int}$ 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.

$$\hat{H}_0 + \hat{H}_{int} = \begin{pmatrix} \Delta E_L & \epsilon \\ \epsilon^* & 0 \end{pmatrix}$$

where the order of the states labeling the rows and columns is

$$\left|2s_{1/2}\right\rangle \left|2p_{1/2}\right\rangle$$

and $\Delta E_L =$ Lamb shift and

$$\epsilon = \left\langle 2p_{1/2}, 1/2\right| \hat{H}_{int} \left|2s_{1/2}, 1/2\right\rangle$$

To calculate ϵ, 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

$$\epsilon = -\sqrt{3}ea_0E_z \text{ (real)}$$

We diagonalize as follows:

$$\hat{H} = \begin{pmatrix} \Delta E_L & 0 \\ 0 & 0 \end{pmatrix} + \hat{H}_0 + \hat{H}_{int} = \epsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

$$|\pm\rangle = \cos\left(\frac{\Theta}{2}\right) \left|2p_{1/2}\right\rangle \pm \sin\left(\frac{\Theta}{2}\right) \left|2s_{1/2}\right\rangle$$

where

$$\tan\Theta = \frac{2\epsilon}{\Delta E_L} \rightarrow \text{ the so-called mixing angle}$$

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

$$\Delta E_L' = E_+ - E_- = \sqrt{(\Delta E_L)^2 + e\epsilon^2}$$

We need to find the electric field such that $\Delta E_L' = 2\Delta E_L$. We get

$$4\epsilon^2 = 3(\Delta E_L)^2 \to \epsilon = \frac{\sqrt{3}}{2}\Delta E_L$$

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 ΔE_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

$$\Delta E_L = (10^9\, Hz)(4.14 \times 10^{-15}\, eV - sec) = 4.14 \times 10^{-6}\, eV$$

Using $a_0 = 0.5 \times 10^{-8}\, cm$ (6.5$\mathring{A}$ we have

$$E_z = \frac{4.14 \times 10^{-6}\, V}{10^{-8}\, cm} = 414 V/cm$$

What about the other substates? There are no off-diagonal matrix elements between different m_j.

PROOF:

$$\left\langle 2s_{1/2}, 1/2 \right| \hat{H}_{int} \left| 2p_{1/2}, -1/2 \right\rangle = eE_z \left[\frac{\sqrt{1}}{3} \langle 2s, 0| \hat{z} |2p, 0\rangle \langle 1/2 \,|\, -1/2\rangle - \frac{\sqrt{2}}{3} \langle 2s, 0| \hat{z} |2p, -1\rangle \langle 1/2 \,|\, 1/2\rangle \right]$$

Using $\langle 1/2 \,|\, -1/2\rangle = 0$ and $\langle 2s, 0| \hat{z} |2p, -1\rangle = 0$ we get

$$\left\langle 2s_{1/2}, 1/2 \right| \hat{H}_{int} \left| 2p_{1/2}, -1/2 \right\rangle = 0$$

and similarly

$$\left\langle 2s_{1/2}, -1/2 \right| \hat{H}_{int} \left| 2p_{1/2}, 1/2 \right\rangle = 0$$

The 2×2 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

$$\hat{H} = \begin{pmatrix} \Delta E_L & \epsilon & \vdots & 0 & 0 \\ \epsilon & 0 & \vdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \vdots & \Delta E_L & \epsilon \\ 0 & 0 & \vdots & \epsilon & 0 \end{pmatrix}$$

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 $0\,GHz < x < 10\,GHz$.

Comment on the behavior of these curves. Do they have the expected asymptotic behavior? Find analytically the eigenvectors in the limit $x/\Delta E_{FS} \to \infty$. Show that these are the expected perturbed states.

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 bo $p \to p$ matrix elements for parity reasons, i.e., $\langle 2p, m_j | \hat{z} | 2p, m_j' \rangle = 0$.

Therefore, we must diagonalize the following 3×3 matrix

$$\hat{H} = \begin{pmatrix} \Delta E_L & \epsilon & \beta \\ \epsilon & 0 & 0 \\ \beta & 0 & \Delta E_{FS} \end{pmatrix} \qquad m_j = \pm 1/2$$

where the row/column order is

$$|2s_{1/2}\rangle \quad |2p_{1/2}\rangle \quad |2p_{3/2}\rangle$$

Note that $Ket2p_{3/2}, m_j = \pm 3/2$ is *unperturbed*.

We have

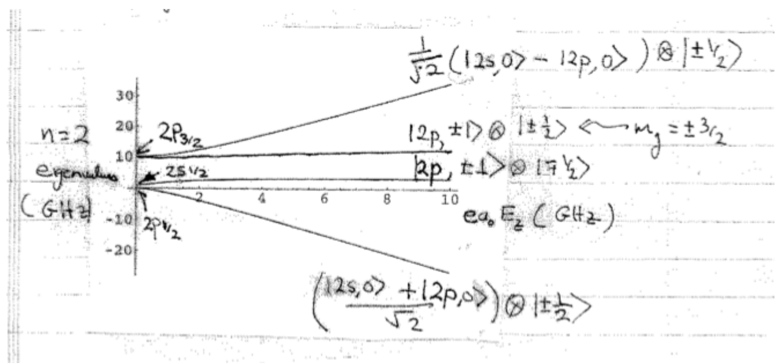
$$\begin{aligned} \beta &= \langle 2p_{3/2}, 1/2 | \hat{H}_{int} | 2s_{1/2}, 1/2 \rangle \\ &- eE_z \left[\sqrt{\frac{2}{3}} \langle 2p, 0 | \hat{z} | 2s, 0 \rangle \langle 1/2 \,|\, 1/2 \rangle + \sqrt{\frac{1}{3}} \langle 2p, 1 | \hat{z} | 2s, 0 \rangle \langle -1/2 \,|\, 1/2 \rangle \right] \\ &= \sqrt{6} e a_0 E_z \end{aligned}$$

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 $\Delta E_L = 1\,GHz$.

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 $\left|2p_{3/2}\right\rangle$ 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

$$|e_1\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} -\sqrt{3} \\ 1 \\ \sqrt{2} \end{pmatrix} \quad |e_2\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 \\ -\sqrt{2} \\ 1 \end{pmatrix} \quad |e_3\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} \\ 1 \\ \sqrt{2} \end{pmatrix}$$

in the ordered basis

$$\left|2s_{1/2}\right\rangle \quad \left|2p_{1/2}\right\rangle \quad \left|2p_{3/2}\right\rangle \quad m_j = 1/2$$

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.

Note the $m_j = -1/2$ are the same asymptotes with $m_s \to -m_s$ and the $m_j = -3/2$ are flat throughout and yield the remaining states $|2p,\pm 1\rangle \otimes |\pm 1/2\rangle$.

8.9.27 2-Particle Ground State Energy

Estimate the ground state energy of a system of two interacting particles of mass m_1 and m_2 with the interaction energy

$$U(\vec{r}_1 - \vec{r}_2) = C\left(|\vec{r}_1 - \vec{r}_2|^4\right)$$

using the variational method.

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

$$\psi(\vec{r}) = R(r)Y_{00}(\theta,\phi) = Ae^{-\alpha r^2}Y_{00}(\theta,\phi)$$

Then, normalizing we have

$$A^2 \int e^{-2\alpha r^2} r^2 dr = 1 \to A^2 = \frac{4(2\alpha)^{3/2}}{\sqrt{\pi}}$$

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

$$\nabla^2 R(r) = \frac{1}{r}\frac{\partial^2}{\partial r^2}(rR(r)) = A\frac{1}{r}\frac{\partial^2}{\partial r^2}(re^{-\alpha r^2}) = A(4\alpha^2 r^2 - 6\alpha)e^{-\alpha r^2}$$

Therefore,

$$\langle H \rangle = -\frac{\hbar^2}{2\mu}A^2\left[-6\alpha\int e^{-2\alpha r^2} r^2 dr + 4\alpha^2\int e^{-2\alpha r^2} r^4 dr\right]$$

$$\langle H \rangle = \frac{3}{2}\frac{\hbar^2}{\mu}\alpha + \frac{15C}{16\alpha^2}$$

We set

$$\frac{\partial\langle H \rangle}{\partial\alpha} = 0$$

to find the value of α that corresponds to the minimum energy. We have

$$\frac{\partial\langle H \rangle}{\partial\alpha} = 0 = \frac{3}{2}\frac{\hbar^2}{\mu} - \frac{30C}{16\alpha^3} \to \alpha^3 = \frac{5\mu C}{\hbar^2}$$

which give an estimated ground state energy of

$$\langle H \rangle = \frac{3}{2}\frac{\hbar^2}{\mu}\left(\frac{5\mu C}{\hbar^2}\right)^{1/3} + \frac{15C}{16}\left(\frac{5\mu C}{\hbar^2}\right)^{-2/3} = 2.42\frac{\hbar^{4/3}C^{1/3}}{\mu^{2/3}}$$

or using a different trial function...

We have

$$H = \frac{p^2}{2\mu} + V(r)$$

where $r = |\vec{r}_1 - \vec{r}_2|$, $V(r) = Cr^4$ and $\mu = m_1 m_2/(m_1 + m_2)$,

We use a trial function

$$\psi(\vec{r}) = R(r)Y_{00}(\theta, \phi) = Ae^{-\alpha r}Y_{00}(\theta, \phi)$$

Then, normalizing we have

$$A^2 \int e^{-2\alpha r} r^2 dr = 1 \rightarrow A^2 = 4\alpha)^3$$

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

$$\nabla^2 R(r) = \frac{1}{r} \frac{\partial^2}{\partial r^2}(rR(r)) = A \frac{1}{r} \frac{\partial^2}{\partial r^2}(re^{-\alpha r}) = A \left(\alpha^2 e^{-\alpha r} - \frac{2\alpha}{r} e^{-\alpha r} \right)$$

Therefore,

$$\langle H \rangle = -\frac{\hbar^2}{2\mu} A^2 \left[-2\alpha \int e^{-2\alpha r} r^d r + \alpha^2 \int e^{-2\alpha r} r^2 dr \right]$$

$$\langle H \rangle = \frac{\hbar^2}{2\mu} \alpha^2 + \frac{45C}{2\alpha^4}$$

We set

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0$$

to find the value of α 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

$$\langle H \rangle = \frac{\hbar^2}{2\mu} \left(\frac{90\mu C}{\hbar^2} \right)^{1/3} + \frac{45C}{2} \left(\frac{90\mu C}{\hbar^2} \right)^{-2/3} = 3.36 \frac{\hbar^{4/3} C^{1/3}}{\mu^{2/3}}$$

Thus, the *Gaussian* trial function yields a lower value for $\langle H \rangle$.

8.9.28 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 ψ_{1s} and ψ_{2s} are both eigenfunctions of H_0 and the energies of ψ_S and ψ_T are equal.

The first-order corrections differ by

$$\begin{aligned}\Delta &= \langle\psi_S|\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}|\psi_S\rangle - \langle\psi_T|\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}|\psi_T\rangle \\ &= 2\langle\psi_{1s}(\vec{r}_1)\psi_{2s}(\vec{r}_2)|\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}|\psi_{1s}(\vec{r}_2)\psi_{2s}(\vec{r}_1)\rangle \\ &= 2\left(\frac{8}{\pi a_0^3}\right)\left(\frac{1}{4\pi a_0^3}\right)e^2\int\int d^3r_1 d^3r_2\left(2 - \frac{2r_1}{a_0}\right)\left(2 - \frac{2r_2}{a_0}\right)\frac{e^{-3(r_1+r_2)/a_0}}{|\vec{r}_1 - \vec{r}_2|}\end{aligned}$$

Now

$$\frac{1}{|\vec{r}_1 - \vec{r}_2|} = \sum_\ell \frac{r_<^\ell}{r_>^{\ell+1}}\frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta_1, \phi_1)Y_{\ell m}^*(\theta_2, \phi_2)$$

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

$$\begin{aligned}
\Delta &= 2(4\pi)^2 \left(\frac{8}{\pi a_0^3}\right)\left(\frac{1}{4\pi a_0^3}\right) e^2 \int_0^\infty r_1^2 dr_1 \left(2 - \frac{2r_1}{a_0}\right) e^{-3r_1/a_0} \int_0^\infty r_2^2 dr_2 \left(2 - \frac{2r_2}{a_0}\right) e^{-3r_2/a_0} \frac{1}{r_>} \\
&= \frac{128e^2}{a_0^6} \int_0^\infty r_1^2 dr_1 \left(2 - \frac{2r_1}{a_0}\right) e^{-3r_1/a_0} \int_{r_1}^\infty r_2^2 dr_2 \left(2 - \frac{2r_2}{a_0}\right) e^{-3r_2/a_0} \frac{1}{r_2} \\
&= \frac{64}{729} \frac{e^2}{a_0} = 2.39\, eV
\end{aligned}$$

8.9.29 Hyperfine Interaction in the Hydrogen Atom

Consider the interaction

$$H_{hf} = \frac{\mu_B \mu_N}{a_B^3} \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2}$$

where μ_B , μ_N are the Bohr magneton and the nuclear magneton, a_B is the Bohr radius, and $\vec{S}_1$, $\vec{S}_2$ are the proton and electron spin operators.

(a) Show that H_{hf} splits the ground state into two levels:

$$E_t = -1\ Ry + \frac{A}{4} \quad , \quad E_s = -1\ Ry - \frac{3A}{4}$$

and that the corresponding states are triplets and singlets, respectively.

Instead of the $|S_1 m_1, S_2, m_2\rangle$ basis ($|m_1 m_2\rangle = |{+}{+}\rangle , |{+}{-}\rangle , ...$), use the total spin (total J) basis $\{|Sm\rangle\} = |1,1\rangle , |1,0\rangle , |1,-1\rangle , |0,0\rangle$.

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

$$\vec{S}_1^2 \to \hbar^2 \left(\frac{1}{2}\right)\left(\frac{1}{2} + 1\right) = \frac{3}{4}\hbar^2 = \vec{S}_2^2$$

Both of these operators are simply *constants* (i.e., times the identity) throughout this Hilbert space.

We get the allowed S values by

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1 \to S = 0, 1$$

and in the $|Sm\rangle$ basis: $\vec{S}^2 \to \hbar^2 S(S+1)$ 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

$$S = 1 \;\; triplet \quad E_t = -1\,Ry + \frac{A}{4}$$

$$S = 0 \;\; singlet \quad E_s = -1\,Ry - \frac{3A}{4}$$

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 $A = \dfrac{\mu_B \mu_N}{a_B^2}$; $\quad \mu_B = g_e \dfrac{e\hbar}{2mc}(g_e = 2), \mu_N = g_N \dfrac{e\hbar}{2Mc}(g_N = 5.6)$

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

$$\frac{e^2\hbar^2}{a_B^2 4mMc^2} = \frac{m}{4M}\alpha^2 \frac{e^2}{a_B} \approx 0.18 \times 10^{-6}\,eV$$

Thus the splitting is $A = 2.09x10^{-6}\,eV$. Now $1\,eV \leftrightarrow \lambda = 1.24 \times 10^4\,cm$. Therefore this splitting corresponds to

$$\lambda_{hf} = \frac{1.24 \times 10^4}{2.09x10^{-6}} = 59.3\,cm$$

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 $B\vec{S}_1 \cdot \vec{S}_2$. 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

$$\Delta E = \frac{4g_p\hbar^4}{3M_p m_e^2 c^2 a_0^4} = 5.88 \times 10^{-6}\, eV$$

which in frequency is $\nu = 1420\, MHz$, and in wavelength is $21\, cm$ - the famous $21\, cm$ line seen in spectra emanating from interstellar space.

8.9.30 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:

$$\langle \mathbf{1}00|\, d_1^q\, |\mathbf{2}im\rangle \rightarrow \langle \mathbf{1}0\|d\|\mathbf{2}1\rangle\, \langle 00\,|\, 1q; 1m\rangle$$

(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-Gordon coefficients.

First, convert $\vec{d} \leftrightarrow d_1^q$. We have

$$d_1^0 = d_z \quad , \quad d_1^{\pm 1} = \mp\frac{1}{\sqrt{2}}(d_x \pm i d_y)$$

We then have for the p_x, p_y, p_z orbitals

$$\psi_{210} = C\frac{r}{a_0}e^{-r/2a_0}\cos\theta \equiv p_z \quad C = \left(\frac{1}{32\pi a_0^3}\right)^{1/2}$$

$$\begin{aligned}\psi_{21\pm1} &= \mp\frac{C}{\sqrt{2}}\frac{r}{a_0}e^{-r/2a_0}\sin\theta e^{\pm i\phi} \\ &\mp C\frac{r}{a_0}e^{-r/2a_0}\left(\sin\theta\left(\frac{\cos\phi \pm i\sin\phi}{\sqrt{2}}\right)\right) \equiv \mp\frac{p_x \pm ip_y}{\sqrt{2}}\end{aligned}$$

We then have

$$p_x = \frac{1}{\sqrt{2}}(-\psi_{211} + \psi_{21-1}) \quad p_y = -\frac{i}{\sqrt{2}}(\psi_{211} + \psi_{21-1})$$

(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 (ℓ, m) indices).

Normalizing properly we have

$$\psi_{210} = R_{21}(r)Y_{10} \quad , \quad Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$$

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

$$\langle 1s|\,\vec{d}\,|2p_x\rangle = \left(\int R_{1s}^*(-er)R_{2p}r^2dr\right)\langle Y_{00}|\,\hat{d}\,|2p_x\rangle$$

The value of the radial integral is

$$\int R_{1s}^*(-er)R_{2p}r^2dr = -\frac{4!}{\sqrt{6}}\left(\frac{2}{3}\right)^5 ea_0$$

(c) Reconstruct the vector matrix elements.

$$\langle 1s|\,\vec{d}\,|2p_j\rangle$$

and discuss the angular dependence you find.

Putting things together, the result is , using

$$D = -\frac{4!}{\sqrt{6}}\left(\frac{2}{3}\right)^5 ea_0$$

$$\langle 1s|\,\vec{d}\,|2p_x\rangle = (D,0,0)\ ,\ \langle 1s|\,\vec{d}\,|2p_y\rangle = (0,D,0)\ ,\ \langle 1s|\,\vec{d}\,|2p_z\rangle = (0,0,D)$$

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.

8.9.31 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

$$\begin{aligned}\langle\psi_\alpha|\,\hat{H}\,|\psi_\alpha\rangle &= \int_{-\infty}^{\infty} dx\psi_\alpha(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\psi_\alpha(x) \\ &= \frac{\hbar^2}{2m}\sqrt{\frac{\pi\alpha}{2}} + \frac{1}{8}m\omega^2\sqrt{\frac{\pi}{2\alpha^3}}\end{aligned}$$

Therefore,

$$\bar{H}_\alpha = \frac{\hbar^2}{2m}\alpha + \frac{1}{8}m\omega^2\frac{1}{\alpha}$$

Then we have

$$\frac{d\bar{H}_\alpha}{d\alpha} = 0 \to \frac{\hbar^2}{2m} - \frac{1}{8}m\omega^2\frac{1}{\alpha^2}$$

or

$$\alpha_{min} = \frac{m\omega}{2\hbar}$$

Thus,

$$\psi_{\alpha_{min}}(x) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-m\omega x^2/2\hbar} \quad , \quad \bar{H}_{min} = \frac{\hbar\omega}{2}$$

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

$$\langle \psi_\alpha \mid \psi_\alpha \rangle = \frac{\pi}{2\alpha^{3/2}}$$

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

$$\frac{d\bar{H}_\alpha}{d\alpha} = 0 \rightarrow \alpha_{min} = \frac{\hbar}{\sqrt{2} m\omega}$$

and therefore

$$\bar{H}_{min} = \frac{\hbar\omega}{\sqrt{2}}$$

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:

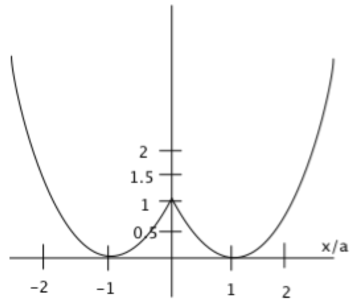


Figure 8.6: Double Oscillator Potential

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

$$\begin{aligned} A_n &= \int u_n(x-a)\hat{H}u_n(x-a)dx \\ B_n &= \int u_n(x-a)\hat{H}u_n(x+a)dx \\ C_n &= \int u_n(x+a)\hat{H}u_n(x-a)dx \end{aligned}$$

In this case, the variational estimate is the mean value since we have no parameter to minimize. Thus,

$$E_n^{(\pm)} = \frac{\left\langle \psi_n^{(\pm)} \middle| \hat{H} \middle| \psi_n^{(\pm)} \right\rangle}{\left\langle \psi_n^{(\pm)} \middle| \psi_n^{(\pm)} \right\rangle}$$

Now

$$\left\langle \psi_n^{(\pm)} \middle| \psi_n^{(\pm)} \right\rangle = \left\langle u_n^{(+)} \middle| u_n^{(+)} \right\rangle + \left\langle u_n^{(-)} \middle| u_n^{(-)} \right\rangle + 2\left\langle u_n^{(+)} \middle| u_n^{(-)} \right\rangle = 1+2+2C_n$$

where $u_n^{(\pm)} = u_n(x \mp a) = \left\langle x \middle| u_n^{(\pm)} \right\rangle$ and

$$\begin{aligned}\left\langle \psi_n^{(\pm)} \right| \hat{H} \left| \psi_n^{(\pm)} \right\rangle &= \left\langle u_n^{(+)} \right| \hat{H} \left| u_n^{(+)} \right\rangle + \left\langle u_n^{(-)} \right| \hat{H} \left| u_n^{(-)} \right\rangle \\ &\pm \left\langle u_n^{(+)} \right| \hat{H} \left| u_n^{(-)} \right\rangle \pm \left\langle u_n^{(-)} \right| \hat{H} \left| u_n^{(+)} \right\rangle \\ &= 2(A_n \pm B_n) \qquad \text{by parity}\end{aligned}$$

Therefore

$$E_n^{\pm} = \frac{A_n \pm B_n}{1 + C_n}$$

(e) For a much larger than the ground state width, show that

$$\Delta E_0 = E_0^{(-)} - E_0^{(+)} \approx 2\hbar\omega \sqrt{\frac{2V_0}{\pi\hbar\omega}} e^{-2V_0/\hbar\omega}$$

where $V_0 = m\omega^2 a^2/2$. This is known as the ground *tunneling* splitting. Explain why?

For the ground state

$$u_0(x) = \left(\frac{\beta}{\pi}\right)^{1/4} e^{-\beta x^2/2} \quad , \quad \beta = \frac{m\omega}{\hbar}$$

The ground state splitting is

$$\Delta E_0 = E_0^{(-)} - E_0^{(+)} = -\frac{2B_0}{1 + C_0}$$

where

$$\begin{aligned}C_0 &= \int_{-\infty}^{\infty} dx u_0(x+a) u_0(x-a) = \sqrt{\frac{\beta}{\pi}} \int_{-\infty}^{\infty} dx e^{-\beta[(x+a)^2 + (x-a)^2]/2} \\ &= e^{-\beta a^2} \sqrt{\frac{\beta}{\pi}} \int_{-\infty}^{\infty} dx e^{-\beta x^2} = e^{-\beta a^2}\end{aligned}$$

and

$$\begin{aligned}B_0 = \int_{-\infty}^{\infty} dx u_0(x+a) \hat{H} u_0(x-a) &= \int_{-\infty}^{0} dx u_0(x+a) \hat{H}_- u_0(x-a) \\ &+ \int_{0}^{\infty} dx u_0(x+a) \hat{H}_+ u_0(x-a)\end{aligned}$$

where

$$\hat{H}_{\pm} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2(x \mp a)^2$$

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

$$\Delta E_0 = 2\hbar\omega\sqrt{\frac{\beta}{\pi}}ae^{-\beta a^2}$$

Noting that

$$\beta a^2 = \frac{m\omega a^2}{\hbar} = \frac{2V_0}{\hbar}$$

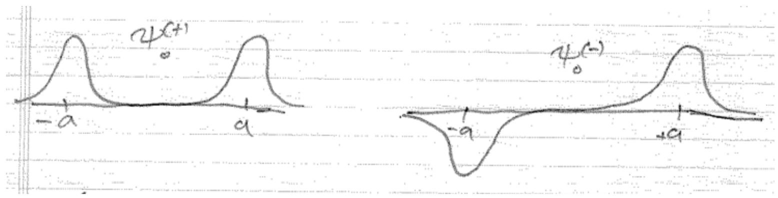
so that

$$\Delta E_0 = 2\hbar\omega\sqrt{\frac{2V_0}{\hbar\omega}}ae^{-2V_0/\hbar\omega}$$

This is known as the *tunneling splitting* since the energy difference determines the frequency of tunneling between the left/right wells, i.e., $\omega_{tunnel} = \Delta E_0/\hbar$.

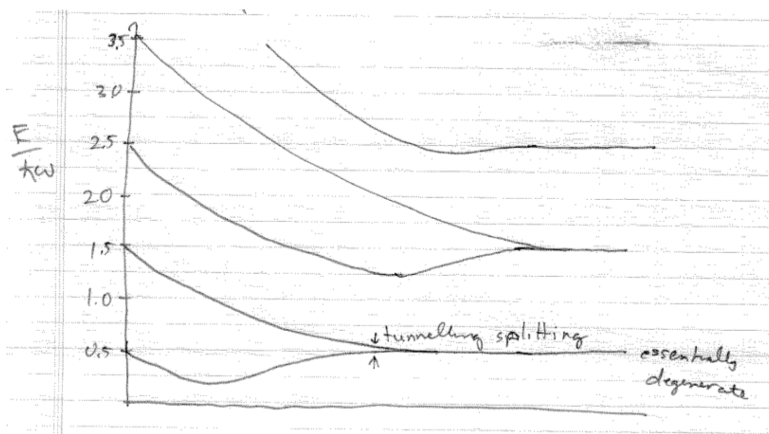
(f) This approximation clearly breaks down as $a \to 0$. Think about the limits and sketch the energy spectrum as a function of a.

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



8.9.32 Variational Method 2

For a particle in a box that extends from $-a$ to $+a$, try the trial function (within the box)

$$\psi(x) = (x-a)(x+a)$$

and calculate E. There is no parameter to vary, but you still get an upper bound. Compare it to the true energy. Convince yourself that the singularities in ψ'' at $x = \pm a$ do not contribute to the energy.

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,

$$E_0 \leq \frac{\langle\psi| H |\psi\rangle}{\langle\psi \mid \psi\rangle} = \frac{-\frac{\hbar^2}{2m}\int\limits_{-a}^{a} dx(x-a)(x+a)\frac{d^2}{dx^2}(x-a)(x+a)}{\int\limits_{-a}^{a} dx(x-a)^2(x+a)^2}$$

$$E_0 \leq \frac{-\frac{\hbar^2}{2m}2\int\limits_{-a}^{a} dx(x^2-a^2)}{\int\limits_{-a}^{a} dx(x^2-a^2)^2} = \frac{-\frac{\hbar^2}{m}\left[\frac{x^3}{3}-a^2x\right]_{-a}^{a}}{\left[\frac{x^5}{5}-\frac{2a^2x^3}{3}+a^4x\right]_{-a}^{a}} = \frac{\frac{\hbar^2}{m}\frac{4}{3}a^3}{\frac{16}{15}a^5}$$

$$E_0 \leq \frac{5}{4}\frac{\hbar^2}{ma^2} = 1.25\frac{\hbar^2}{ma^2}$$

The exact solution gives the result

$$E_{0,exact} = \frac{\pi^2}{8}\frac{\hbar^2}{ma^2} = 1.2325\frac{\hbar^2}{ma^2}$$

so $E_{0,exact} \leq E_0$ as expected.

8.9.33 Variational Method 3

For the attractive delta function potential

$$V(x) = -aV_0\delta(x)$$

use a Gaussian trial function. Calculate the upper bound on E_0 and compare it to the exact answer $-ma^2V_0^2/2h^2$.

For $V(x) = -aV_0\delta(x)$ and the Gaussian trial function $\psi = e^{-\alpha x^2}$ we have

$$E_0 \leq \frac{\langle\psi| H |\psi\rangle}{\langle\psi \mid \psi\rangle} = \frac{-\frac{\hbar^2}{2m}\int\limits_{-\infty}^{\infty} dx e^{-\alpha x^2}\frac{d^2}{dx^2}e^{-\alpha x^2} - aV_0\int\limits_{-\infty}^{\infty} dx e^{-2\alpha x^2}\delta(x)}{\int\limits_{-a}^{a} dx e^{-2\alpha x^2}}$$

$$E_0 \leq \frac{-\frac{\hbar^2}{2m}\int\limits_{-\infty}^{\infty} dx e^{-2\alpha x^2}\left(4\alpha^2x^2-2\alpha\right) - aV_0}{\sqrt{\frac{\pi}{2\alpha}}} = \frac{-\frac{\hbar^2}{2m}\left(\left(4\alpha^2\frac{\sqrt{\pi}}{2(2\alpha)^{3/2}} - 2\alpha\sqrt{\frac{\pi}{2\alpha}}\right)\right) - aV_0}{\sqrt{\frac{\pi}{2\alpha}}}$$

$$E_0 \leq -\sqrt{\frac{2\alpha}{\pi}}\left(aV_0 + \frac{\hbar^2}{2m}\left(\frac{1}{\sqrt{2}}\alpha^{1/2}\sqrt{\pi} - \sqrt{2}\alpha^{1/2}\sqrt{\pi}\right)\right) = -\sqrt{\frac{2\alpha}{\pi}}\left(aV_0 + \frac{\hbar^2}{2m}\alpha^{1/2}\sqrt{\pi}\left(\frac{1}{\sqrt{2}} - \sqrt{2}\right)\right)$$

Now,

$$\frac{dE_0}{d\alpha} = 0 \rightarrow -\sqrt{\frac{2}{\pi}}\left(\frac{1}{2}aV_0\alpha^{-1/2} + \frac{\hbar^2}{2m}\sqrt{\pi}\left(\frac{1}{\sqrt{2}} - \sqrt{2}\right)\right)$$

$$\alpha^{1/2} = \frac{aV_0}{\frac{\hbar^2}{m}\sqrt{\pi}\left(\sqrt{2}-\frac{1}{\sqrt{2}}\right)} = \frac{maV_0\sqrt{2}}{\hbar^2\sqrt{\pi}}$$

so that

$$E_0 \leq -\sqrt{\frac{2\alpha}{\pi}}\left(aV_0 + \frac{\hbar^2}{2m}\alpha^{1/2}\sqrt{\pi}\left(\frac{1}{\sqrt{2}} - \sqrt{2}\right)\right) = -\frac{maV_0\sqrt{2}}{\hbar^2\sqrt{\pi}}\sqrt{\frac{2}{\pi}}\left(aV_0 - \frac{\hbar^2}{2m}\frac{maV_0}{\hbar^2\sqrt{\pi}}\sqrt{\pi}\right)$$
$$E_0 \leq -\frac{ma^2V_0^2}{\pi\hbar^2} = -0.318\frac{ma^2V_0^2}{\hbar^2}$$

The exact result is

$$E_{0,exact} = -0.500\frac{ma^2V_0^2}{\hbar^2} < E_0$$

as expected.

8.9.34 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 $V(x) = m\omega^2x^2/2$. Now we have

$$\int_{-a}^{a} \psi^*\psi dx = 0.81a^9$$
$$\int_{-a}^{a} \psi^* V(x)\psi dx = 0.70m\omega^2a^{11}$$
$$-\frac{\hbar^2}{2m}\int_{-a}^{a} \psi^*\frac{d^2}{dx^2}\psi dx = 1.23\frac{\hbar^2}{2m}a^7$$

Therefore,

$$E_0 \leq \frac{1.23\frac{\hbar^2}{2m}a^7 + 0.70m\omega^2a^{11}}{0.81a^9} = 1.52\frac{\hbar^2}{ma^2} + 0.86m\omega^2a^2$$

Minimizing, we have

$$\frac{dE_0}{da} = 0 \to a^2 = 1.33\frac{\hbar}{m\omega}$$

so that

$$E_0 \leq 2.28\hbar\omega$$

The exact answer is

$$E_{0,exact} = 0.50\hbar\omega < E_0$$

as expected.

8.9.35 Variation on a linear potential

Consider the energy levels of the potential $V(x) = g\,|x|$.

(a) By dimensional analysis, reason out the dependence of a general eigenvalue on the parameters $m = mass$, $\hbar$ and g.

The Schrodinger equation is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + g\,|x|\right)\psi(x) = E\psi(x) \rightarrow \left(\frac{d^2}{dx^2} + \frac{2m}{\hbar^2}\left(E - g\,|x|\right)\right)\psi(x) = 0$$

Since

$$\left[\frac{mE}{\hbar^2}\right] = L^{-2} \quad , \quad \left[\frac{mg}{\hbar^2}\right] = L^{-3} \rightarrow \left[\frac{mE}{\hbar^2}\right]^3 \leftrightarrow \left[\frac{mg}{\hbar^2}\right]^2 \rightarrow E \propto \left(\frac{\hbar^2}{m}g^2\right)^{1/3}$$

or the eigenvalues have the form

$$E_n = \left(\frac{\hbar^2}{m}g^2\right)^{1/3} f(n)$$

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

$$\langle H \rangle = \int \psi^*(x)\hat{H}\psi(x)dx = \int \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + g\,|x|\right)\psi(x)dx$$
$$= -\frac{\hbar^2}{2m}\int \psi^*(x)\frac{d^2\psi(x)}{dx^2}dx + g\int \psi^*(x)\,|x|\,\psi(x)dx$$

Now,

$$\int \psi^*(x)\,|x|\,\psi(x)dx = |c|^2\left(-\int_{-a}^{0} x\left(1+\frac{x}{a}\right)^2 dx + \int_{0}^{q} x\left(1-\frac{x}{a}\right)^2 dx\right) = \frac{a^2}{b}\,|c|^2 = \frac{a}{4}$$

and

$$\frac{d\psi}{dx} = c\delta(x+a)\theta(a-x)\left(1-\frac{|x|}{a}\right) - c\theta(x+a)\delta(a-x)\left(1-\frac{|x|}{a}\right) + c\theta(x+a)\theta(a-x)\left(-\frac{|x|}{x}\frac{1}{a}\right)$$

Therefore, we have

$$\int \psi(x)\frac{d^2\psi(x)}{dx^2}dx = \psi(x)\frac{d\psi(x)}{dx}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left(\frac{d\psi(x)}{dx}\right)^2 dx = -\int_{-\infty}^{\infty}\left(\frac{d\psi(x)}{dx}\right)^2 dx$$

$$\int \psi^*(x)\frac{d^2\psi(x)}{dx^2}dx = -|c|^2\int_{-a}^{a}\left(\frac{|x|}{x}\frac{1}{a}\right)^2 dx = -\frac{2|c|^2}{a} = -\frac{3}{a^2}$$

and thus

$$\langle H\rangle = \frac{3\hbar^2}{2ma^2} + \frac{ga}{4}$$

For its minimum value we have

$$\frac{d}{da}\langle H\rangle = 0 = -\frac{3\hbar^2}{ma^3} + \frac{g}{4} \to a = \left(\frac{12\hbar^2}{mg}\right)^{1/3}$$

so that the estimate of the ground state energy is

$$\langle H\rangle = \frac{3\hbar^2}{2m\left(\frac{12\hbar^2}{mg}\right)^{2/3}} + \frac{g\left(\frac{12\hbar^2}{mg}\right)^{1/3}}{4} = \frac{3}{4}\left(\frac{3\hbar^2 g^2}{2m}\right)^{1/3}$$

(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

$$1 = \int \psi^*(x)\psi(x)dx = 2a\,|c|^2 \to |c|^2 = \frac{1}{2a}$$
$$\int \psi(x)\frac{d^2\psi(x)}{dx^2}dx = 0$$
$$\int \psi^*(x)\,|x|\,\psi(x)dx = a^2\,|c|^2 = \frac{a}{2}$$

so that

$$\langle H\rangle = \frac{ga}{2} \to \frac{d}{da}\langle H\rangle = 0 = \frac{g}{2} \neq 0$$

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.

8.9.36 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 ℓ, but not on s and j.

We denote the common eigenbasis of H_0, L^2, S^2, and J^2 by $\{|n\ell s; jm_j\rangle\}$.

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

$$\begin{aligned}
&(2(\ell+1/2)+1)\frac{1}{2}A((\ell+1/2)(\ell+3/2) - \ell(\ell+1) - 3/4) \\
&\quad + (2(\ell-1/2)+1)\frac{1}{2}A((\ell-1/2)(\ell+1/2) - \ell(\ell+1) - 3/4) \\
&\quad = A\ell^2 + A\ell - A\ell - A\ell^2 = 0
\end{aligned}$$

8.9.37 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:

$$\begin{array}{l} |n_x n_y n_z; \pm\rangle \rightarrow E^{(0)}_{n_x n_y n_z} = (n_x + n_y + n_z + 3/2)\,\hbar\omega \\ ground - state \rightarrow n_x = n_y = n_z = 0 \end{array}$$

Now since $E^{(1)}_{\pm} = \langle 000; \pm| V |000; \pm\rangle = 0$ 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

$$0 = \det \begin{vmatrix} \sum\limits_{m \neq |000;\pm\rangle} \frac{V_{000+,m}V_{m,000+}}{E^{(0)}_{000} - E^{(0)}_m} - E & \sum\limits_{m \neq |000;\pm\rangle} \frac{V_{000+,m}V_{m,000-}}{E^{(0)}_{000} - E^{(0)}_m} \\ \sum\limits_{m \neq |000;\pm\rangle} \frac{V_{000-,m}V_{m,000+}}{E^{(0)}_{000} - E^{(0)}_m} & \sum\limits_{m \neq |000;\pm\rangle} \frac{V_{000-,m}V_{m,000-}}{E^{(0)}_{000} - E^{(0)}_m} - E \end{vmatrix}$$

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

$$\begin{array}{l} \lambda \langle 000; \pm| (\hat{\sigma}_x x) |100; \mp\rangle \\ or \\ \lambda \langle 000; \pm| (\hat{\sigma}_y y) |010; \mp\rangle \\ or \\ \lambda \langle 000; \pm| (\hat{\sigma}_z z) |001; \pm\rangle \end{array}$$

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

$$\langle\pm|\,\hat{\sigma}_x\,|\mp\rangle = 1 \quad , \quad \langle\pm|\,\hat{\sigma}_y\,|\mp\rangle = \mp i \quad , \quad \langle\pm|\,\hat{\sigma}_z\,|\pm\rangle = \pm 1$$

Therefore,

$$\sum_{m\neq|000;\pm\rangle} \frac{V_{000+,m}V_{m,000+}}{E^{(0)}_{000}-E^{(0)}_{m}} = -\frac{\lambda^2}{\hbar\omega}(1+1+1)\frac{\hbar}{2m\omega} = -\frac{3\lambda^2}{2m\omega^2} = \sum_{m\neq|000;\pm\rangle} \frac{V_{000-,m}V_{m,000-}}{E^{(0)}_{000}-E^{(0)}_{m}}$$

$$\sum_{m\neq|000;\pm\rangle} \frac{V_{000+,m}V_{m,000-}}{E^{(0)}_{000}-E^{(0)}_{m}} = -\frac{\lambda^2}{\hbar\omega}(0) = 0 = \sum_{m\neq|000;\pm\rangle} \frac{V_{000-,m}V_{m,000+}}{E^{(0)}_{000}-E^{(0)}_{m}}$$

We get a diagonal result so that the degeneracy remains to second-order and we have

$$E_{000} = \frac{3}{2}\hbar\omega - \frac{3\lambda^2}{2m\omega^2}$$

8.9.38 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 Schrodinger 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 $R(r) = \chi(r)/r$, $\ell = 0$ 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

$$E_{10} = -\frac{me^4}{2\hbar^2} \quad , \quad \chi_{10}(r) = \frac{2r}{a_0^{3/2}} e^{-r/a_0} \quad , \quad a_0 = \frac{\hbar^2}{me^2}$$

become

$$E_1^{(0)} = -\frac{mK^2}{2\hbar^2} \quad , \quad \psi_1^{(0)}(x) = \frac{2x}{a^{3/2}} e^{-x/a} \quad , \quad a = \frac{\hbar^2}{mK}$$

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

$$E_1^{(1)} = \left\langle \psi_1^{(0)} \middle| V \middle| \psi_1^{(0)} \right\rangle = \frac{4e\varepsilon}{a^3} \int_0^\infty x^3 e^{-2x/a} dx = \frac{3}{2} e\varepsilon a = \frac{3e\varepsilon\hbar^2}{2mK}$$

8.9.39 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

$$\psi_{100}(\vec{r}) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{2a_0}\right)^{3/2} e^{-r/2a_0} \quad , \quad a_0 = \frac{\hbar^2}{me^2}$$

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

$$\left\langle r^2 \right\rangle = \frac{1}{8\pi a_0^3} \int_0^\infty e^{-r/a_0} r^4 dr = \frac{a_0^2}{8\pi} \int_0^\infty e^{-x} x^4 dx = \frac{3a_0^2}{\pi}$$

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

$$\vec{\mu} = \frac{ge}{2mc}\hat{\vec{S}}$$

Using first order perturbation theory compute the energy difference between the singlet and triplet ground states. Determine which lies lowest. Express the energy splitting in GHz. Get a number!

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 enrgy correction

$$\begin{aligned}
\Delta E &= \langle 1, 0, 0, s', s_z'| \hat{H}_{\text{int}} |1, 0, 0, s, s_z\rangle \\
&= -\frac{8\pi}{3} \int d^3r \psi_{100}^*(\vec{r})\delta(\vec{r})\psi_{100}(\vec{r}) \langle s', s_z'| \vec{\mu}_e \cdot \vec{\mu}_p |s, s_z\rangle \\
&= -\frac{8\pi}{3} \left(\frac{ge}{2mc}\right)^2 |\psi_{100}(0)|^2 \langle s', s_z'| \hat{S}_e \cdot \hat{S}_p |s, s_z\rangle
\end{aligned}$$

Now,

$$\hat{S}_e \cdot \hat{S}_p = \frac{1}{2}\left(S^2 - S_e^2 - S_p^2\right) = \frac{\hbar^2}{2}\left(S(S+1) - 3/2\right)$$

and therefore is diagonal in this basis. We then have

$$\Delta E = -\frac{8\pi}{3}\left(\frac{ge}{2mc}\right)^2 \left(\frac{1}{2a_0}\right)^3 \frac{\hbar^2}{2}\left(S(S+1) - 3/2\right)$$

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

$$\Delta E_0 = 2\pi\left(\frac{e}{mc}\right)^2 \left(\frac{1}{2a_0}\right)^3 \hbar^2 = \frac{1}{4}\left(\frac{e^2}{\hbar c}\right)^2 \frac{e^2}{a_0} = \frac{1}{4}mc^2\alpha^4 > 0$$

For the triplet state

$$\Delta E_1 = -\frac{1}{12}\left(\frac{e^2}{\hbar c}\right)^2 \frac{e^2}{a_0} = -\frac{1}{12}mc^2\alpha^4 < 0$$

Thus, the triplet ground state has the lowest energy and the energy splitting of the perturbed ground state levels is

$$\Delta E_0 - \Delta E_1 = \Delta E = \frac{1}{3}mc^2\alpha^4 = \frac{1}{3}\left(0.51\times 10^6\,eV\right)\left(\frac{1}{137}\right)^4 = 4.83\times 10^{-4}\,eV$$

corresponding to

$$\frac{\Delta E}{\hbar} = \nu = 1.17\times 10^{11}\,Hz = 117\,GHz$$

8.9.40 Two coupled spins

Two oppositely charged spin$-1/2$ particles (spins $\vec{s}_1 = \hbar\vec{\sigma}_1/2$ and $\vec{s}_2 = \hbar\vec{\sigma}_2/2$) are coupled in a system with a spin-spin interaction energy ΔE. The system is placed in a uniform magnetic field $\vec{B} = B\hat{z}$. The Hamiltonian for the spin interaction is

$$\hat{H} = \frac{\Delta E}{4}\vec{\sigma}_1\cdot\vec{\sigma}_2 - (\vec{\mu}_1 + \vec{\mu}_2)\cdot\vec{B}$$

where $\vec{\mu}_j = g_j\mu_0\vec{s}_j/\hbar$ is the magnetic moment of the j^{th} particle.

(a) If we define the 2-particle basis-states in terms of the 1-particle states by

$$|1\rangle = |+\rangle_1|+\rangle_2 \quad , \quad |2\rangle = |+\rangle_1|-\rangle_2 \quad , \quad |3\rangle = |-\rangle_1|+\rangle_2 \quad , \quad |4\rangle = |-\rangle_1|-\rangle_2$$

where

$$\sigma_{ix}|\pm\rangle_i = |\mp\rangle_i \quad , \quad \sigma_{ix}|\pm\rangle_i = \pm i|\mp\rangle_i \quad , \quad \sigma_{iz}|\pm\rangle_i = \pm|\pm\rangle_i$$

and

$$\sigma_{1x}\sigma_{2x}|1\rangle = \sigma_{1x}\sigma_{2x}|+\rangle_1|+\rangle_2 = (\sigma_{1x}|+\rangle_1)(\sigma_{2x}|+\rangle_2) = |-\rangle_1|-\rangle_2 = |4\rangle$$

then derive the results below.

The energy eigenvectors for the 4 states of the system, in terms of the eigenvectors of the $z-$component of the operators $\vec{\sigma}_{\rm i} = 2\vec{s}_i/\hbar$ are

$$|1'\rangle = |+\rangle_1|+\rangle_2 = |1\rangle \quad , \quad |2'\rangle = d|-\rangle_1|+\rangle_2 + c|+\rangle_1|-\rangle_2 = d|3\rangle + c|2\rangle$$
$$|3'\rangle = c|-\rangle_1|+\rangle_2 - dc|+\rangle_1|-\rangle_2 = c|3\rangle - d|2\rangle \quad , \quad |4'\rangle = |-\rangle_1|-\rangle_2 = |4\rangle$$

where

$$\vec{\sigma}_{\rm zi}|\pm\rangle_i = \pm|\pm\rangle_i$$

as stated above and

$$d = \frac{1}{\sqrt{2}}\left(1 - \frac{x}{\sqrt{1+x^2}}\right)^{1/2} \;,\; c = \frac{1}{\sqrt{2}}\left(1 + \frac{x}{\sqrt{1+x^2}}\right)^{1/2} \;,\; x = \frac{\mu_0 B(g_2 - g_1)}{\Delta E}$$

(b) Find the energy eigenvalues associated with the 4 states.

We have

$$\vec{\mu} = g_i \mu_0 \vec{S}_i \quad , \quad \vec{S}_i = \frac{\hbar}{2}\vec{\sigma}_i \quad , \quad \vec{B} = B\hat{z}$$

$$\begin{aligned}\hat{H} &= \frac{\Delta E}{4}\vec{\sigma}_1 \cdot \vec{\sigma}_2 - (\vec{\mu}_1 + \vec{\mu}_2)\cdot \vec{B} \\ &= \frac{\Delta E}{4}\left(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}\right) - \frac{1}{2}\mu_0 B\left(g_1\sigma_{1z} + g_2\sigma_{2z}\right)\end{aligned}$$

In the $\hat{\sigma}_z$ basis, we have 1-particle states with these properties

$$\begin{aligned}&\hat{\sigma}_x \left|+\right\rangle = \left|-\right\rangle \quad , \quad \hat{\sigma}_x \left|-\right\rangle = \left|+\right\rangle \\ &\hat{\sigma}_y \left|+\right\rangle = i\left|-\right\rangle \quad , \quad \hat{\sigma}_y \left|-\right\rangle = -i\left|+\right\rangle \\ &\hat{\sigma}_z \left|+\right\rangle = \left|+\right\rangle \quad , \quad \hat{\sigma}_z \left|-\right\rangle = -\left|-\right\rangle\end{aligned}$$

We now define the 2-particle basis

$$\left|1\right\rangle = \left|+\right\rangle_1 \left|+\right\rangle_2 \quad , \quad \left|2\right\rangle = \left|+\right\rangle_1 \left|-\right\rangle_2 \quad , \quad \left|3\right\rangle = \left|-\right\rangle_1 \left|+\right\rangle_2 \quad , \quad \left|4\right\rangle = \left|-\right\rangle_1 \left|-\right\rangle_2$$

We then have

$$\begin{aligned}&\hat{\sigma}_{1x}\hat{\sigma}_{2x}\left|1\right\rangle = \hat{\sigma}_{1x}\hat{\sigma}_{2x}\left|+\right\rangle_1\left|+\right\rangle_2 = \hat{\sigma}_{1x}\left|+\right\rangle_1\hat{\sigma}_{2x}\left|+\right\rangle_2 = \left|-\right\rangle_1\left|-\right\rangle_2 = \left|4\right\rangle \\ &\hat{\sigma}_{1x}\hat{\sigma}_{2x}\left|2\right\rangle = \left|3\right\rangle \quad , \quad \hat{\sigma}_{1x}\hat{\sigma}_{2x}\left|3\right\rangle = \left|2\right\rangle \quad , \quad \hat{\sigma}_{1x}\hat{\sigma}_{2x}\left|4\right\rangle = \left|1\right\rangle \\ &\hat{\sigma}_{1y}\hat{\sigma}_{2y}\left|1\right\rangle = -\left|4\right\rangle \quad , \quad \hat{\sigma}_{1y}\hat{\sigma}_{2y}\left|2\right\rangle = \left|3\right\rangle \quad , \quad \hat{\sigma}_{1y}\hat{\sigma}_{2y}\left|3\right\rangle = \left|2\right\rangle \quad , \quad \hat{\sigma}_{1y}\hat{\sigma}_{2y}\left|4\right\rangle = -\left|1\right\rangle \\ &\hat{\sigma}_{1z}\hat{\sigma}_{2z}\left|1\right\rangle = \left|1\right\rangle \quad , \quad \hat{\sigma}_{1z}\hat{\sigma}_{2z}\left|2\right\rangle = -\left|2\right\rangle \quad , \quad \hat{\sigma}_{1z}\hat{\sigma}_{2z}\left|3\right\rangle = -\left|3\right\rangle \quad , \quad \hat{\sigma}_{1z}\hat{\sigma}_{2z}\left|4\right\rangle = \left|4\right\rangle \\ &\hat{\sigma}_{1z}\left|1\right\rangle = \left|1\right\rangle \quad , \quad \hat{\sigma}_{1z}\left|2\right\rangle = \left|2\right\rangle \quad , \quad \hat{\sigma}_{1z}\left|3\right\rangle = -\left|3\right\rangle \quad , \quad \hat{\sigma}_{1z}\left|4\right\rangle = -\left|4\right\rangle \\ &\hat{\sigma}_{2z}\left|1\right\rangle = \left|1\right\rangle \quad , \quad \hat{\sigma}_{2z}\left|2\right\rangle = -\left|2\right\rangle \quad , \quad \hat{\sigma}_{2z}\left|3\right\rangle = \left|3\right\rangle \quad , \quad \hat{\sigma}_{2z}\left|4\right\rangle = -\left|4\right\rangle\end{aligned}$$

Then

$$\begin{aligned}&\hat{H}\left|1\right\rangle = \left(\tfrac{\Delta E}{4} - \tfrac{1}{2}\mu_0 B(g_1+g_2)\right)\left|1\right\rangle \\ &\to H_{11} = \tfrac{\Delta E}{4} - \tfrac{1}{2}\mu_0 B(g_1+g_2)\ ,\ H_{12} = H_{21} = H_{13} = H_{31} = H_{14} = H_{41} = 0\end{aligned}$$

$$\begin{aligned}&\hat{H}\left|2\right\rangle = \left(-\tfrac{\Delta E}{4} - \tfrac{1}{2}\mu_0 B(g_1-g_2)\right)\left|2\right\rangle + \tfrac{\Delta E}{2}\left|3\right\rangle \\ &\to H_{22} = -\tfrac{\Delta E}{4} - \tfrac{1}{2}\mu_0 B(g_1-g_2)\ ,\ H_{12} = H_{21} = H_{24} = H_{42} = 0\ ,\ H_{23} = H_{32} = \tfrac{\Delta E}{2}\end{aligned}$$

$$\begin{aligned}&\hat{H}\left|3\right\rangle = \left(-\tfrac{\Delta E}{4} + \tfrac{1}{2}\mu_0 B(g_1-g_2)\right)\left|3\right\rangle + \tfrac{\Delta E}{2}\left|2\right\rangle \\ &\to H_{33} = -\tfrac{\Delta E}{4} + \tfrac{1}{2}\mu_0 B(g_1-g_2)\ ,\ H_{13} = H_{31} = H_{34} = H_{43} = 0\ ,\ H_{23} = H_{32} = \tfrac{\Delta E}{2}\end{aligned}$$

$$\begin{aligned}&\hat{H}\left|4\right\rangle = \left(\tfrac{\Delta E}{4} + \tfrac{1}{2}\mu_0 B(g_1+g_2)\right)\left|4\right\rangle \\ &\to H_{44} = \tfrac{\Delta E}{4} + \tfrac{1}{2}\mu_0 B(g_1+g_2)\ ,\ H_{14} = H_{41} = H_{24} = H_{42} = H_{34} = H_{43} = 0\end{aligned}$$

We then have the $\hat{H}$ matrix in the 2-particle basis

$$H = \begin{pmatrix} \frac{\Delta E}{4} - \frac{\mu_0 v}{2}(g_1+g_2) & 0 & 0 & 0 \\ 0 & -\frac{\Delta E}{4} - \frac{\mu_0 B}{2}(g_1-g_2) & \frac{\Delta E}{2} & 0 \\ 0 & \frac{\Delta E}{2} & -\frac{\Delta E}{4} + \frac{\mu_0 B}{2}(g_1-g_2) & 0 \\ 0 & 0 & 0 & \frac{\Delta E}{4} + \frac{\mu_0 B}{2}(g_1+g_2) \end{pmatrix}$$

Eigenvalues: We already have two diagonal elements so that

$$E_1 = \frac{\Delta E}{4} - \frac{1}{2}\mu_0 B(g_1 + g_2) \quad , \quad E_4 = \frac{\Delta E}{4} + \frac{1}{2}\mu_0 B(g_1 + g_2)$$

We obtain the characteristic equation for the other two eigenvalues from the 2×2 matrix. We have

$$\left(-\frac{\Delta E}{4} - \frac{1}{2}\mu_0 B(g_1 - g_2) - E\right)\left(-\frac{\Delta E}{4} + \frac{1}{2}\mu_0 B(g_1 - g_2) - E\right) - \left(\frac{\Delta E}{2}\right)^2 = 0$$

$$E^2 + \frac{\Delta E}{2}E + \left(\frac{\Delta E}{4}\right)^2 - \frac{1}{4}(\mu_0 B(g_1 - g_2))^2 - \left(\frac{\Delta E}{2}\right)^2 = 0$$

$$\begin{aligned} E_\pm &= -\frac{\Delta E}{4} \pm \frac{1}{2}\sqrt{\left(\frac{\Delta E}{2}\right)^2 + (\mu_0 B(g_1 - g_2))^2 + \frac{3}{4}(\Delta E)^2} \\ &= -\frac{\Delta E}{4}\left(1 \mp 2\sqrt{1 + x^2}\right) \end{aligned}$$

where

$$x = \frac{\mu_0 B(g_1 - g_2)}{\Delta E}$$

Eigenvectors: We then have the following complete solution

$$\begin{aligned} &|\bar{1}\rangle = |1\rangle \to E_1 = \tfrac{\Delta E}{4} - \tfrac{1}{2}\mu_0 B(g_1 + g_2) \\ &|\bar{2}\rangle = d\,|3\rangle + c\,|2\rangle \to E_2 = -\tfrac{\Delta E}{4}\left(1 - 2\sqrt{1 + x^2}\right) \\ &|\bar{3}\rangle = d\,|3\rangle - c\,|2\rangle \to E_3 = -\tfrac{\Delta E}{4}\left(1 + 2\sqrt{1 + x^2}\right) \\ &|\bar{4}\rangle = |4\rangle \to E_4 = \tfrac{\Delta E}{4} + \tfrac{1}{2}\mu_0 B(g_1 + g_2) \end{aligned}$$

where

$$c^2 + d^2 = 1 \quad , \quad \langle \bar{2} \mid \bar{3}\rangle = 0 \; (orthogonal)$$

Now we can determine c and d as follows.

$$\begin{aligned} &\hat{H}\,|\bar{2}\rangle = E_2\,|\bar{2}\rangle \\ &\hat{H}\,(d\,|3\rangle + c\,|2\rangle) = -\tfrac{\Delta E}{4}\left(1 - 2\sqrt{1 + x^2}\right)(d\,|3\rangle + c\,|2\rangle) \end{aligned}$$

$$\begin{aligned} &d\left(\left(-\frac{\Delta E}{4} + \frac{1}{2}\mu_0 B(g_1 - g_2)\right)|3\rangle + \frac{\Delta E}{2}\,|2\rangle\right) + c\left(\left(-\frac{\Delta E}{4} - \frac{1}{2}\mu_0 B(g_1 - g_2)\right)|2\rangle + \frac{\Delta E}{2}\,|3\rangle\right) \\ &\quad = -\frac{\Delta E}{4}\left(1 - 2\sqrt{1 + x^2}\right)(d\,|3\rangle + c\,|2\rangle) \end{aligned}$$

$$\begin{aligned} &\to d - \left(\tfrac{1}{2} + x\right)c = -\tfrac{1}{2}\left(1 - 2\sqrt{1 + x^2}\right)c \\ &\to c - \left(\tfrac{1}{2} - x\right)d = \tfrac{1}{2}\left(1 - 2\sqrt{1 + x^2}\right)d \end{aligned}$$

We then find

$$c = \frac{1}{\sqrt{2}}\left(1 + \frac{x}{\sqrt{1 + x^2}}\right)^{1/2} \quad , \quad d = \frac{1}{\sqrt{2}}\left(1 - \frac{x}{\sqrt{1 + x^2}}\right)^{1/2}$$

(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

$$\begin{aligned}
E_1 &= \tfrac{\Delta E}{4} - \tfrac{1}{2}\mu_0 B(g_1+g_2) \\
E_2 &= -\tfrac{\Delta E}{4}\left(1 - 2\sqrt{1+x^2}\right) = -\tfrac{\Delta E}{4}\left(-1-x^2\right) = -\tfrac{\Delta E}{4}\left(-1-\left(\tfrac{\mu_0 B(g_1-g_2)}{\Delta E}\right)^2\right) \\
E_3 &= -\tfrac{\Delta E}{4}\left(1 + 2\sqrt{1+x^2}\right) = -\tfrac{\Delta E}{4}\left(2+x^2\right) = -\tfrac{\Delta E}{4}\left(2+\left(\tfrac{\mu_0 B(g_1-g_2)}{\Delta E}\right)^2\right) \\
E_4 &= \tfrac{\Delta E}{4} + \tfrac{1}{2}\mu_0 B(g_1+g_2)
\end{aligned}$$

so that in the limit $x \to 0$ we have

$$\begin{aligned}
E_1 &= \tfrac{\Delta E}{4} = E_2 = E_4 \\
E_3 &= -\tfrac{3\Delta E}{4}
\end{aligned}$$

or two distinct levels (one is 3-fold degenerate).

For $\mu_0 B/\Delta E >> 1$ or $x \gg 1$ we have

$$\begin{aligned}
E_1 &= \tfrac{\Delta E}{4} - \tfrac{1}{2}\mu_0 B(g_1+g_2) = -\tfrac{1}{2}\mu_0 B(g_1+g_2) \\
E_2 &= -\tfrac{\Delta E}{4}\left(1 - 2\sqrt{1+x^2}\right) = -\tfrac{\Delta E}{4}\left(-2x\right) = \tfrac{\mu_0 B(g_1-g_2)}{2} \\
E_3 &= -\tfrac{\Delta E}{4}\left(1 + 2\sqrt{1+x^2}\right) = -\tfrac{\Delta E}{4}\left(2x\right) = -\tfrac{\mu_0 B(g_1-g_2)}{2} \\
E_4 &= \tfrac{\Delta E}{4} + \tfrac{1}{2}\mu_0 B(g_1+g_2) = \tfrac{1}{2}\mu_0 B(g_1+g_2)
\end{aligned}$$

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

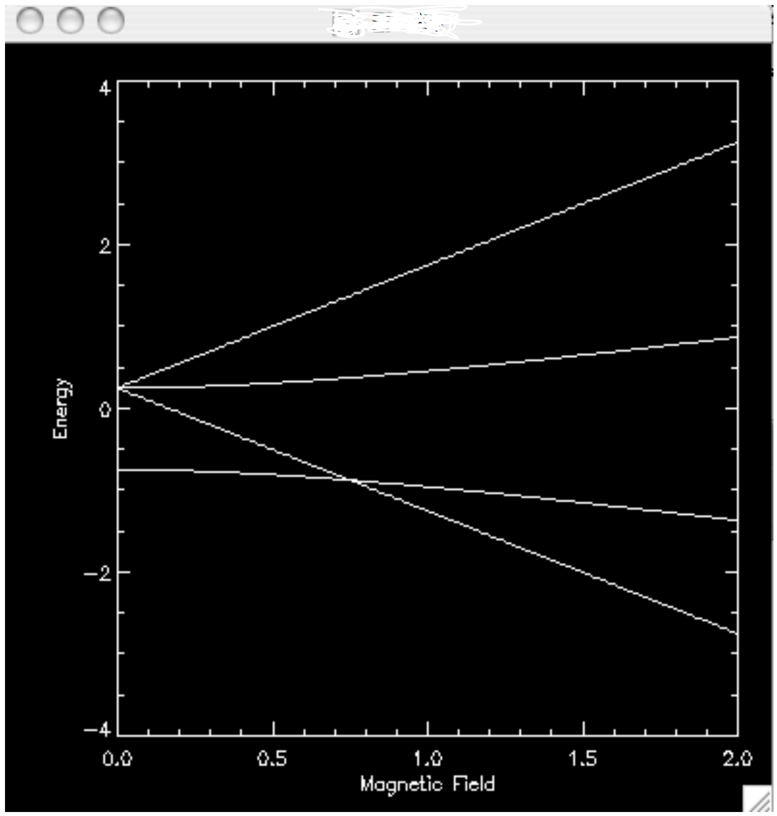
$$\begin{aligned}
E_1 &= \tfrac{1}{4} - \tfrac{3}{2}B \\
E_2 &= -\tfrac{1}{4}\left(1 - 2\sqrt{1+B^2}\right) \\
E_3 &= -\tfrac{1}{4}\left(1 + 2\sqrt{1+B^2}\right) \\
E_4 &= \tfrac{1}{4} + \tfrac{3}{2}B
\end{aligned}$$

as shown below.

8.9.41 Perturbed Linear Potential

A particle moving in one-dimension is bound by the potential

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



where $a > 0$ is a constant. Estimate the ground state energy using first-order perturbation theory by the following method: Write $V = V_0 + V_1$ where $V_0(x) = bx^2$, $V_1(x) = ax - bx^2$ (for $x > 0$), where b is a constant and treat V_1 as a perturbation.

We have

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

where

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

We now write

$$V = V_0 + V_1$$

where

$$V_0(x) = \begin{cases} bx^2 & x > 0 \\ \infty & x < 0 \end{cases}$$

$$V_1(x) = \begin{cases} ax - bx^2 & x > 0 \\ \infty & x < 0 \end{cases}$$

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 $|n\rangle$, $n = 1, 3, 5, ...$ with corresponding energies $E_n^{(0)} = \hbar\omega(n + 1/2)$, $n = 1, 3, 5, ...$

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

$$\begin{aligned} E_n^{(1)} &= \langle n| V_1 |n\rangle /2 \\ &= -bx_0^2 \langle n| (aa^+ + a^+a) |n\rangle /2 = -bx_0^2 \langle n| (2a^+a + 1) |n\rangle /2 \\ &= -bx_0^2(n + 1/2) \quad , \quad n = 1, 3, 5, ... \end{aligned}$$

8.9.42 The ac-Stark Effect

Suppose an atom is perturbed by a monochromatic electric filed oscillating at frequency ω_L, $\vec{E}(t) = E_z \cos\omega_L t \hat{e}_z$ (such as from a linearly polarized laser), rather than the dc-field studied in the text. We know that such a field can be absorbed and cause transitions between the energy levels: we will systematically study this effect in Chapter 11. The laser will also cause a *shift* of energy levels of the unperturbed states, known alternatively as the *ac-Stark effect*, the *light shift*, and sometimes the *Lamp shift* (don't you love physics humor). In this problem, we will look at this phenomenon in the simplest case that the field is near to resonance between the ground state $|g\rangle$ and some excited state $|e\rangle$, $\omega_L \approx \omega_{eg} = (E_e - E_g)/\hbar$, so that we can ignore all other energy levels in the problem (the *two-level atom* approximation).

(i) **The classical picture**. Consider first the *Lorentz oscillator* model of the atom - a charge on a spring - with natural resonance at ω_0. The Hamiltonian for the system is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 z^2 - \vec{d} \cdot \vec{E}(t)$$

where $d = -ez$ is the dipole.

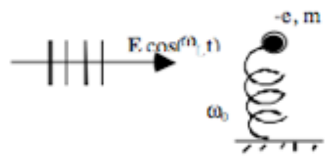


Figure 8.7: Lorentz Oscillator

(a) Ignoring damping of the oscillator, use Newton's Law to show that the induced dipole moment is

$$\vec{d}_{induced}(t) = \alpha\vec{E}(t) = \alpha E_z \cos\omega_L t$$

where

$$\alpha = \frac{e^2/m}{\omega_0^2 - \omega_L^2} \approx \frac{-e^2}{2m\omega_0\Delta}$$

is the polarizability with $\Delta = \omega_L - \omega_0$ the *detuning*.

The incident field will drive oscillations of the charge at frequency ω_L. The equation of motion is

$$\ddot{z} + \omega_0^2 z = -\frac{e}{m} E_z \cos\omega_L t$$

We shift to complex amplitudes via

$$z \equiv \Re(Z_0 e^{-i\omega_L t})$$

This gives

$$(-\omega_L^2 + \omega_0^2) Z_0 = -\frac{e}{m} E_z \rightarrow Z_0 = -\frac{e}{m}\frac{1}{\omega_0^2 - \omega_L^2} E_z$$

The induced dipole moment oscillating at drive-frequency ω_L is

$$d_{induced}(t) = \Re(-eZ_0 e^{-i\omega_L t}) = \frac{e^2}{m}\frac{1}{\omega_0^2 - \omega_L^2} E_z \cos\omega_L t$$

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

$$\Delta \equiv \omega_L - \omega_0$$

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

$$\bar{H} = -\frac{1}{4}\alpha E_z^2$$

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

$$\begin{aligned} H &= \frac{1}{2}m(\omega_0^2 - \omega_L^2)z^2 - \vec{d}\cdot\vec{E} \\ &= \frac{1}{2}m(\omega_0^2 - \omega_L^2)\frac{e^2}{m^2}\frac{1}{\omega_0^2 - \omega_L^2}{}^2 E^2 - \alpha E^2 \\ &= \frac{1}{2}\alpha E^2 - \alpha E^2 = -\frac{1}{2}\alpha E^2 \end{aligned}$$

Therefore,

$$H = -\frac{1}{2}\alpha E^2(t) = -\frac{1}{2}\vec{d}_{ind}(t)\cdot\vec{E}(t)$$

Time averaging using

$$\overline{\cos^2}\omega_L t = \frac{1}{2}$$

we get

$$\bar{H} = -\frac{1}{4}\alpha E_z^2$$

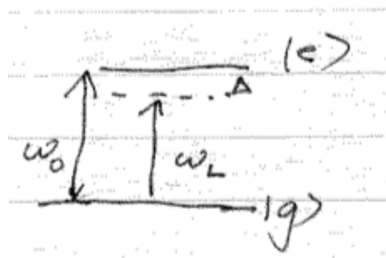
(ii) **The quantum picture**. We consider the two-level atom described above. The Hamiltonian for this system can be written in a time independent form (equivalent to the time-averaging done in the classical case).

$$\hat{H} = \hat{H}_{atom} + \hat{H}_{int}$$

where $\hat{H}_{atom} = -\hbar\Delta\,|e\rangle\langle e|$ is the *unperturbed* atomic Hamiltonian and $\hat{H}_{int} = -\frac{\hbar\Omega}{2}\left(|e\rangle\langle g| + |g\rangle\langle e|\right)$ 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 Δ. 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

$$\hat{H}_0 = \hat{H}_{atom} == \hbar\Delta \left|e\right\rangle \left\langle e\right| \to \text{ the "unperturbed atom"}$$

$$\hat{H}_1 = -\frac{\hbar\Omega}{2}(\left|e\right\rangle \left\langle g\right| + \left|g\right\rangle \left\langle e\right|) \to \text{ the "laser interaction"}$$

with

$$\Omega = \frac{\left\langle e\right| \vec{d} \left|g\right\rangle \cdot \vec{E}}{\hbar} \to \text{ the "Rabi frequency"}$$

This simple 2-dimensional problem can be solved exactly. We can write the matrix representation in the $\{\left|e\right\rangle, \left|g\right\rangle\}$ basis as

$$H = -\hbar \begin{pmatrix} \Delta & \Omega/2 \\ \Omega/2 & 0 \end{pmatrix} = -\hbar \left(\frac{\Delta}{2}\hat{I} + \frac{\Delta}{2}\hat{sigma}_z + \frac{\Omega}{2}\hat{sigma}_x \right)$$
$$= -\hbar\frac{\Delta}{2}\hat{I} - \frac{\hbar}{2}\vec{\bar{\Omega}} \cdot \vec{\sigma}$$

where

$$\vec{\bar{\Omega}} = \Delta\hat{e}_z + \Omega\hat{e}_x$$

is the *generalized Rabi frequency* and

$$\bar{\Omega} \equiv |\vec{\bar{\Omega}}| = \sqrt{\Omega^2 + \Delta^2}$$

so that

$$\frac{\vec{\bar{\Omega}}}{\bar{\Omega}} \equiv \cos\theta\hat{e}_z + \sin\theta\hat{e}_x$$

with

$$\tan\theta = \frac{\Omega}{\Delta}$$

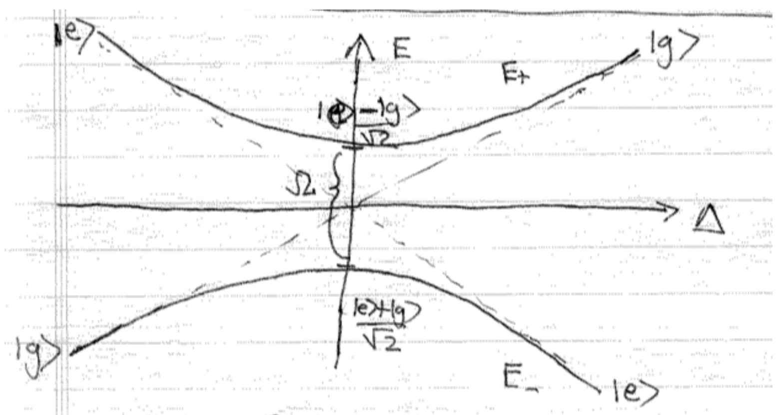
We then have the eigenvalues

$$E_\pm = -\frac{\hbar}{2}(\Delta \pm \bar{\Omega}) = -\frac{\hbar}{2}(\Delta \pm \sqrt{\Omega^2 + \Delta^2})$$

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, Δ is negative.

(b) Expand your solution in (a) to lowest nonvanishing order in Ω to find the perturbation to the energy levels. Under what conditions is this expansion valid?

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

$$E_+ \approx -\hbar\Delta - \frac{\hbar\Omega^2}{4\Delta} \quad , \quad E_- \approx \frac{\hbar\Omega^2}{4\Delta}$$

Thus, the lowest non-vanishing perturbation is *second-order* in Ω.

(c) Confirm your answer to (b) using perturbation theory. Find also the mean induced dipole moment (to lowest order in perturbation theory), and from this show that the atomic polarizability, defined by $\langle\vec{d}\rangle = \alpha\vec{E}$ is given by

$$\alpha = -\frac{|\langle e|\,\vec{d}\,|g\rangle|^2}{\hbar\Delta}$$

so that the second order perturbation to the ground state is $E_g^{(2)} = -\alpha E_z^2$ as in part (b).

Using perturbation theory where

$$\hat{H}_1 = -\frac{\hbar\Omega}{2}(|e\rangle\langle g| + |g\rangle\langle e|)$$

we have

0^{th}−order:

$$E_e^{(0)} = -\hbar\Delta \quad , \quad E_g^{(0)} = 0$$

1^{st}−order:

$$E_e^{(1)} = \langle e|\,\hat{H}_1\,|e\rangle = 0 \quad , \quad E_g^{(1)} = \langle g|\,\hat{H}_1\,|g\rangle = 0$$

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

$$\left|\tilde{\phi}_g\right\rangle = |g\rangle + |e\rangle \frac{\langle e| \hat{H}_1 |g\rangle}{E_g^{(0)} - E_e^{(0)}} = \left|\phi_g^{(0)}\right\rangle + \left|\phi_g^{(1)}\right\rangle$$

Therefore

$$\left|\tilde{\phi}_g\right\rangle = |g\rangle - \frac{\Omega}{2\Delta} |e\rangle \quad \text{(unnormalized)}$$

Thus,

$$\langle \vec{d} \rangle = \frac{\left\langle \tilde{\phi}_g \middle| \vec{d} \middle| \tilde{\phi}_g \right\rangle}{\left\langle \tilde{\phi}_g \middle| \tilde{\phi}_g \right\rangle} = -\frac{1}{2\Delta} \frac{\Omega^* \langle e| \vec{d} |g\rangle + \Omega \langle g| \vec{d} |e\rangle}{1 + \frac{\Omega^2}{4\Delta^2}}$$

Since

$$\frac{\Omega^2}{4\Delta^2} \ll 1$$

we can write

$$\langle \vec{d} \rangle = -\frac{1}{2\Delta} (\Omega^* \langle e| \vec{d} |g\rangle + \Omega \langle g| \vec{d} |e\rangle)$$

Then, to lowest order in

$$\Omega = \frac{\langle e| \vec{d} |g\rangle \cdot \vec{E}}{\hbar}$$

$$\langle \vec{d} \rangle = -\frac{| \langle e| \vec{d} |g\rangle |^2}{\hbar\Delta} \vec{E} = \alpha \vec{E}$$

and

$$E_g^{(2)} = \frac{\hbar\Omega^2}{4\Delta} = \frac{| \langle e| \vec{d} |g\rangle |^2}{4\hbar\Delta} |\vec{E}|^2 = -\frac{1}{4} \alpha |\vec{E}|^2$$

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

$$f = \frac{\alpha_{quantum}}{\alpha_{classical}} = \frac{| \langle e| z |g\rangle |^2}{(\Delta z^2)_{SHO}}$$

where $\left(\Delta z^2\right)_{SHO}$ is the SHO zero point variance. This is also known as the oscillator strength.

We have

$$f = \frac{\alpha_q}{\alpha_c} = \frac{| \langle e| \vec{d} |g\rangle |^2}{\hbar\Delta} \frac{2m\omega_0\Delta}{e^2} = \frac{2m\omega_0}{\hbar} | \langle e| \vec{d} |g\rangle |^2$$

Thus,

$$f = \frac{|\langle e|\,\vec{d}\,|g\rangle\,|^2}{(\Delta z)^2_{SHO}}$$

where

$$(\Delta z)_{SHO} = \frac{\hbar}{2m\omega_0}$$

For a multi-level atom with resonances $\{\omega_i\}$

$$\alpha = \sum_i f(\omega_i)\alpha(\omega_i)$$

The oscillator strentgh satisfies the *sum rule*

$$\sum_i f(\omega_i) = Z \quad \text{(atomic number}$$

For hydrogen and the alkalis, the majority of the oscillator strength lies in the first $s \to p$ 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).

8.9.43 Light-shift for multilevel atoms

We found the ac-Stark (light shift) for the case of a two-level atom driven by a monchromatic field. In this problem we want to look at this phenomenon in a more general context, including arbitrary polarization of the electric field and atoms with multiple sublevels.

Consider then a general monochromatic electric field $\vec{E}(\vec{x},t) = \Re(\vec{E}(\vec{x})e^{-i\omega_L t})$, driving an atom near resonance on the transition $|g; J_g\rangle \to |e; J_e\rangle$, where the ground and excited manifolds are each described by some total angular momentum J with degeneracy $2J+1$. The generalization of the ac-Stark shift is now the light-shift operator acting on the $2J_g+1$ dimensional ground manifold:

$$\hat{V}_{LS}(\vec{x}) = -\frac{1}{4}\vec{E}^*(\vec{x}) \cdot \hat{\overleftrightarrow{\alpha}} \cdot \vec{E}(\vec{x})$$

Here,

$$\hat{\overleftrightarrow{\alpha}} = -\frac{\hat{\vec{d}}_{ge}\hat{\vec{d}}_{eg}}{\hbar\Delta}$$

is the atomic polarizability tensor operator, where $\hat{\vec{d}}_{eg} = \hat{P}_e\hat{\vec{d}}\hat{P}_g$ is the dipole operator, projected between the ground and excited manifolds; the projector onto the excited manifold is

$$\hat{P}_e = \sum_{M_e=-J_e}^{J_e} |e; J_e, M_e\rangle \langle e; J_e, M_e|$$

and similarly for the ground manifold.

(a) By expanding the dipole operator in the spherical basis$(\pm, 0)$, show that the polarizability operator can be written

$$\hat{\vec{\alpha}} = \tilde{\alpha} \left(\begin{array}{c} \sum_{q,M_g} \left| C_{M_g}^{M_g+q} \right|^2 \vec{e}_q \, |g, J_g, M_g\rangle \langle g, J_g, M_g| \, \vec{e}_q^{\;*} \\ + \sum_{q \neq q', M_g} C_{M_g+q-q'}^{M_g+q} \, C_{M_g}^{M_g+q} \, \vec{e}_{q'} \, |g, J_g, M_g + q - q'\rangle \langle g, J_g, M_g| \, \vec{e}_q^{\;*} \end{array} \right)$$

where

$$\tilde{\alpha} = -\frac{|\langle e; J_e \, \|d\| \, g; J_g\rangle|^2}{\hbar\Delta}$$

and

$$C_{M_g}^{M_e} = \langle J_e M_e \,|\, 1q J_g M_g\rangle$$

Explain physically, using dipole selection rules, the meaning of the expression for $\hat{\vec{\alpha}}$.

Let us write the explicit representation in the basis of the magnetic sublevels:

$$\hat{\vec{d}}_{eg} = \hat{P}_e \hat{\vec{d}} \hat{P}_g = \sum_{M_e=-J_e}^{J_e} \sum_{M_g=-J_g}^{J_g} |e; J_e M_e\rangle \langle e; J_e M_e| \, \hat{\vec{d}} |g; J_g M_g\rangle \langle g; J_g M_g|$$

We can then make a spherical basis expansion

$$\hat{\vec{d}} = \sum_q (-1)^q \vec{e}_{-q} \hat{d}_q = \sum_q \vec{e}_q^{\,*} \hat{d}_q$$

which then implies that

$$\hat{\vec{d}}_{eg} = \sum_{M_e, M_g} \vec{e}_q^{\,*} \langle e; J_e M_e| \, \hat{d}_q \, |g; J_g M_g\rangle \, |e; J_e M_e\rangle \langle g; J_g M_g|$$

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

$$\hat{\vec{d}}_{eg} = \sum_{M_g, q} \vec{e}_q^{\,*} C_{M_g}^{M_g+q} \, |e; J_e M_g + q\rangle \langle g; J_g M_g| \, \langle e\|d\|g\rangle$$

where we have used a shorthand for the dipole CG coefficient

$$C_{M_g}^{M_g+q} = \langle J_e M_g + q \,|\, 1q J_g M_g \rangle$$

Similarly,

$$\hat{\vec{d}}_{ge} = \hat{\vec{d}}_{eg}^{+} = \sum_{M_g,q} \vec{e}_q C_{M_g}^{M_g+q} \left|g; J_g M_g\right\rangle \left\langle e; J_e M_g + q\right| \langle e\|d\|g\rangle^*$$

which says that

$$\hat{\vec{d}}_{ge}\hat{\vec{d}}_{eg} = \sum_{M_g,M_g'} \sum_{q,q'} \vec{e}_{q'} \vec{e}_q^{\,*} C_{M_g'}^{M_g'+q'} C_{M_g}^{M_g+q} |\langle e\|d\|g\rangle|^2 \left|g; J_g M_g'\right\rangle \left\langle e; J_e M_g' + q' \,\middle|\, e; J_e M_g + q\right\rangle \left\langle g; J_g M_g\right|$$

Now

$$\left\langle e; J_e M_g' + q' \,\middle|\, e; J_e M_g + q\right\rangle = \delta_{M_g'+q', M_g+q}$$

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,

$$\hat{\vec{d}}_{ge}\hat{\vec{d}}_{eg} = |\langle e\|d\|g\rangle|^2 sum_{M_g} \sum_{q,q'} \vec{e}_{q'} \vec{e}_q^{\,*} C_{M_g+q-q'}^{M_g+q} C_{M_g}^{M_g+q} \left|g; J_g M_g + q - q'\right\rangle \left\langle g; J_g M_g\right|$$

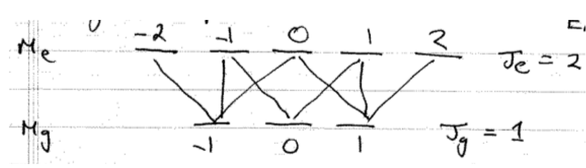
Putting this together, the polarizability tensor in a spherical basis representation is (explicitly writing the diagonal and off-diagonal terms):

$$\hat{\tilde{\alpha}} = \tilde{\alpha} \left(\begin{array}{l} \sum_{q,M_g} \left| C_{M_g}^{M_g+q} \right|^2 \vec{e}_q \left|g, J_g, M_g\right\rangle \left\langle g, J_g, M_g\right| \vec{e}_q^{\;*} \\ \quad + \sum_{q\neq q', M_g} C_{M_g+q-q'}^{M_g+q} C_{M_g}^{M_g+q} \vec{e}_{q'} \left|g, J_g, M_g + q - q'\right\rangle \left\langle g, J_g, M_g\right| \vec{e}_q^{\;*} \end{array} \right)$$

where

$$\tilde{\alpha} = -\frac{|\langle e; J_e \|d\| g; J_g\rangle|^2}{\hbar\Delta}$$

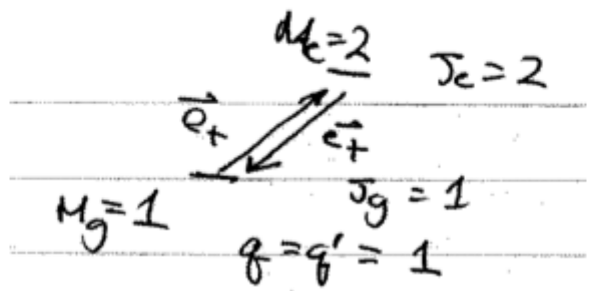
Physical Picture: We have this example(shown below)



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 absrobs a photon of helicty q and emits q', the deficit goes into atomic angular momentum.

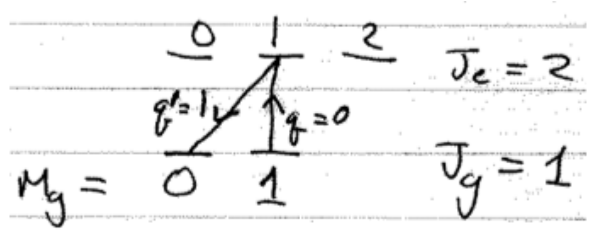
Example-diagonal term:



here the strength is

$$|C^{M_e=2}_{M_g=1}|^2$$

Example-off diagonal term:



here the strength is

$$(C^1_0 C^1_1)$$

(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 $|g;J_g = 1/2\rangle \to |e;J_e = 3/2\rangle$ and comment.

In the plane-polarized case

$$\vec{E}(\vec{x}) = E_1 \vec{\epsilon}_L^* \cdot \hat{\tilde{\alpha}} \cdot \vec{\epsilon}_L$$

which implies that

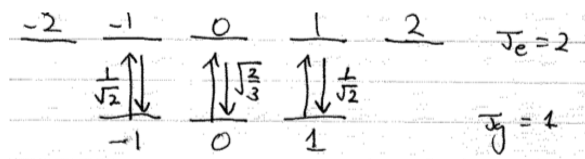
$$\hat{V}_{LS} = -\frac{1}{4}|E_1|^2 \vec{\epsilon}_L^* \cdot \hat{\tilde{\alpha}} \cdot \vec{\epsilon}_L$$

case (i): we have linear polarization along $z : \vec{\epsilon}_L = \vec{\epsilon}_0$. This implies that

$$\hat{V}_{LS} = -\frac{1}{4}|E_1|^2 \vec{\epsilon}_0 \cdot \hat{\tilde{\alpha}} \cdot \vec{\epsilon}_0 = -\frac{\tilde{\alpha}}{4}|E_1|^2 \sum_{M_g} |C_{M_g}^{M_g}|^2 \left| g;J_g M_g \right\rangle \left\langle g;J_g M_g \right|$$

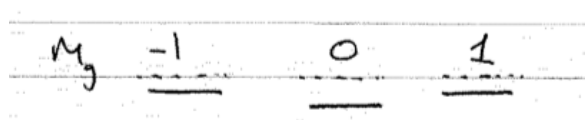
Thus, we only have diagonal terms(as in the figure above)

case (ii): we have $|g;J_g = 1\rangle \to |e;J_e = 2\rangle$ as shown below:

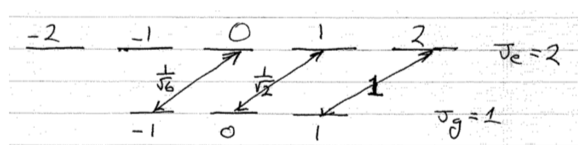


Here the relevant CG coefficients are $C_{M_e}^{M_g} = \langle 2M_g \,|\, 101M_g \rangle$ which implies for $\vec{epsilon}_L = \vec{\epsilon}_z$, that $|J_g = 1\rangle \to |J_e = 2\rangle$.

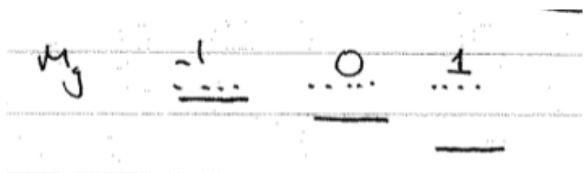
The appropriate eigenvectors are the magnetic sublevels $|g;J_g\rangle$ and the corresponding eigenvalues are $V_1/2, 2V_1/3$. For $\Delta < 0$ which implies $V_1 < 0$ we have the shifted levels



case : $\vec{\epsilon}_L = \vec{\epsilon}_+$ **or** $|J_g = 1\rangle \to |J_e = 2\rangle$ we have



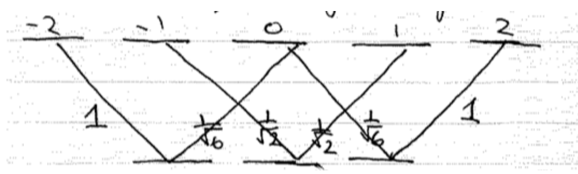
The appropriate eigenvectors are $|J_g, M_g\rangle$ with eigenvalues $M_g = 1 : V_1/6$, $M_g = 0 : V_1/2$, $M_g = +1 : V_1$ with the shifted($V_1 < 0$) level diagram below



case: $\vec{\epsilon}_L = \vec{\epsilon}_x$ **or** $|J_g = 1\rangle \to |J_e = 2\rangle$ 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 $\vec{\epsilon}_L = \vec{\epsilon}_x = (-\vec{e}_+ + \vec{e}_-)/\sqrt{2}$

$$\begin{aligned}
\hat{V}_L(\vec{x}) &= V_1 \sum_{M_g,q} |C_{M_g}^{M_g+q}|^2 (\vec{e}_x \cdot \vec{e}_q) \, |M_g\rangle \langle M_g| \, (\vec{e}_q^{\,*} \cdot \vec{e}_x) \\
&= \quad +V_1 \sum_{M_g q q'} C_{M_g+q-q'}^{M_g+q} C_{M_g}^{M_g+q} (\vec{e}_x \cdot \vec{e}_{q'}) \, |M_g + q - q'\rangle \langle M_g| \, (\vec{e}_{q'}^{\,*} \cdot \vec{e}_x) \\
&= \frac{V_1}{2} \left(\sum_{M_g} (|C_{M_g}^{M_g+1}|^2 + |C_{M_g}^{M_g-1}|^2) \, |M_g\rangle \langle M_g| - \sum_{M_g} (|C_{M_g+2}^{M_g+1}|^2 + |C_{M_g}^{M_g+1}|^2) \, |M_g + 2\rangle \langle M_g| + H.C. \right) \\
&= \frac{V_1}{2} \left(|0\rangle \langle 0| + \frac{1}{12} (7 \, |1\rangle \langle 1| + 7 \, |-1\rangle \langle -1| - |1\rangle \langle -1| - |-1\rangle \langle 1|) \right)
\end{aligned}$$

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:

$$\hat{V}_L = \frac{V_1}{2} \begin{pmatrix} 1 & \vdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & \vdots & \frac{7}{12} & -\frac{1}{12} \\ 0 & \vdots & -\frac{1}{12} & \frac{7}{12} \end{pmatrix}$$

Since this is block-diagonal, we need only diagonalize the 2×2 matrix. It has eigenvalues $)1/2, 2/3)$. Therefore, the eigenvalues/eigenvectors for $\vec{\epsilon}_L = \vec{\epsilon}_x$, $|J_g = 1\rangle \to |J_e = 2\rangle$ are:

$$\frac{V_1}{2} \qquad |0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\frac{V_1}{2} \qquad \frac{|1\rangle + |-1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

$$\frac{2V_1}{3} \qquad \frac{|1\rangle - |-1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

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 $|M_x\rangle = \hat{D} |M_z\rangle$ 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,

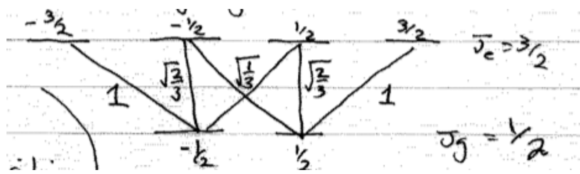
$$\begin{aligned} |1, M_x = 0\rangle &= -\tfrac{1}{\sqrt{2}} \left(|1, M_z = +1\rangle - |1, M_z = -1\rangle\right) \\ |1, M_x = \pm 1\rangle &= -\tfrac{i}{\sqrt{2}} \left(\pm |1, M_z = 0\rangle + \tfrac{1}{\sqrt{2}} |1, M_z = +1\rangle + |1, M_z = -1\rangle\right) \end{aligned}$$

Thus,

$$\begin{aligned} \hat{V}_L |1, M_x = 0\rangle &= \tfrac{2}{3} V_1 |1, M_x = 0\rangle \\ \hat{V}_L |1, M_x = \pm 1\rangle &= \tfrac{1}{2} V_1 |1, M_x = \pm 1\rangle \end{aligned}$$

so it all makes sense.

Let us repeat this for the case: $|g; J_g = 1/2\rangle \to |e; J_e = 3/2\rangle$ as shown below (with CG coefficiuents for dipole transitions):
case (i): $\vec{\epsilon}_L = \vec{\epsilon}_z$. We have eigenvectors $|J_g, M_g = \pm 1/2\rangle$ with eigenvalues $2V_1/3$ (doubly degenerate).



case (ii): $\vec{\epsilon}_L = \vec{\epsilon}_+$. We have eigenvectors $|J_g, M_g = \pm 1/2\rangle$ with eigenvalues $|J_g, M_g = +1/2\rangle \quad V_1$ and $|J_g, M_g = -1/2\rangle \quad V_1/3$.

case (ii): $\vec{\epsilon}_L = (-\vec{\epsilon}_+ + \vec{\epsilon}_-)/\sqrt{2}$. 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 $\vec{\epsilon}_L = \vec{\epsilon}_z$ 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

$$\hat{\alpha}^{(0)} = \frac{\hat{\vec{d}}_{ge} \cdot \hat{\vec{d}}_{eg}}{-3\hbar\Delta} \quad , \quad \hat{\alpha}^{(1)} = \frac{\hat{\vec{d}}_{ge} \times \hat{\vec{d}}_{eg}}{-2\hbar\Delta}$$

and

$$\hat{\alpha}_{ij}^{(2)} = \frac{1}{-\hbar\Delta} \left(\frac{\hat{\vec{d}}_{ge}^{i} \hat{\vec{d}}_{ge}^{j} + \hat{\vec{d}}_{ge}^{j} \hat{\vec{d}}_{ge}^{i}}{2} - \hat{\alpha}^{(0)} \delta_{ij} \right)$$

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.,

$$\hat{T}_{ij} = \hat{T}_{ij}^{(0)} + \hat{T}_{ij}^{(1)} + \hat{T}_{ij}^{(2)}$$

where

$$\hat{T}_{ij}^{(0)} = Trace(\hat{T}_{ij})\frac{\delta_{ij}}{3} = \frac{1}{3}\hat{\vec{d}}^{i}_{ge} \cdot \hat{\vec{d}}^{j}_{eg}$$

$$\hat{T}_{ij}^{(1)} = \frac{\hat{d}^{i}_{ge}\hat{d}^{j}_{eg} - \hat{d}^{j}_{ge}\hat{d}^{i}_{eg}}{2} = \frac{1}{2}\epsilon_{ijk}(\hat{\vec{d}}^{i}_{ge} \times \hat{\vec{d}}^{j}_{eg})_k \quad \text{antyisymmetric}$$

$$\hat{T}_{ij}^{(2)} = \frac{\hat{d}^{i}_{ge}\hat{d}^{j}_{eg} + \hat{d}^{j}_{ge}\hat{d}^{i}_{eg}}{2} = \frac{1}{2}\epsilon_{ijk}(\hat{\vec{d}}^{i}_{ge} \times \hat{\vec{d}}^{j}_{eg})_k - \frac{1}{3}\hat{\vec{d}}^{i}_{ge} \cdot \hat{\vec{d}}^{j}_{eg} \quad \text{symmetric and traceless}$$

Thus, with

$$\hat{\alpha}_{ij} = -\frac{1}{\hbar\Delta}\hat{T}_{ij}$$

we arrive at the desired expansion

$$\begin{aligned}\hat{V}_{LS} &= -\frac{1}{4}\vec{E}^*(\vec{x}) \cdot \hat{\alpha} \cdot \vec{E}(\vec{x}) = -\frac{1}{4}E_i^* E_j \hat{\alpha}_{ij} \\ &= -\frac{1}{4}(\hat{\alpha}^{(0)}|\vec{E}(\vec{x})|^2 + \hat{\alpha}^{(1)} \cdot (\vec{E}^* \times \vec{E}) + \vec{E}^*(\vec{x}) \cdot \hat{\alpha}^{(2)} \cdot \vec{E}(\vec{x})\end{aligned}$$

where

$$\hat{\alpha}^{(k)} = -\frac{1}{\hbar\Delta}\hat{T}_{ij}^{(k)}$$

(d) For the particular case of $|g; J_g = 1/2\rangle \to |e; J_e = 3/2\rangle$, show that the rank-2 tensor part vanishes. Show that the light-shift operator can be written in a basis independent form of a scalar interaction (independent of sublevel), plus an effective Zeeman interaction for a fictitious B-field interacting with the spin$-1/2$ ground state,

$$\hat{V}_{LS} = V_0(\vec{x})\hat{I} + \vec{B}_{fict}(\vec{x}) \cdot \hat{\vec{\sigma}}$$

where

$$V_0(\vec{x}) = \frac{2}{3}U_1|\vec{\varepsilon}_L(\vec{x})|^2 \rightarrow \text{ proportional to field intensity}$$

and

$$\vec{B}_{fict}(\vec{x}) = \frac{1}{3}U_1\left(\frac{\vec{\varepsilon}_L{}^*(\vec{x}) \times \vec{\varepsilon}_L(\vec{x})}{i}\right) \rightarrow \text{ proportional to field ellipticity}$$

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 $|g; J_g = 1/2\rangle \to |e; J_e = 3/2\rangle$.

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

$$\hat{V}_{LS}^{(2)} = -\frac{1}{4}E_i^* E_j \hat{\alpha}_{ij}^{(2)}$$

has matrix elements

$$\left\langle J_g = 1/2, M'_g \right| \hat{V}_{LS}^{(2)} \left| J_g = 1/2, M_g \right\rangle = \langle 1/2 \| \hat{V}_{LS}^{(2)} \| 1/2 \rangle \left\langle 1/2 M'_g \right| 2q1/2M_g \rangle$$

where the CG coefficient $\left\langle 1/2M'_g \right| 2q1/2M_g \rangle$ vanishes by the triangle inequality. Thus,

$$-\frac{1}{4}(\hat{\alpha}^{(0)}|\vec{E}(\vec{x})|^2 + \hat{\alpha}^{(1)} \cdot (\vec{E}^* \times \vec{E})$$

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

$$V_0(\vec{x}) = \frac{1}{2}Tr(\hat{V}_{LS}) \quad , \quad \vec{B}_{eff}(\vec{x}) = \frac{1}{2}Tr(\hat{V}_{LS})\hat{\vec{\sigma}})$$

8.9.44 A Variational Calculation

Consider the one-dimensional box potential given by

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

Use the variational principle with the trial function

$$\psi(x) = |a|^\lambda - |x|^\lambda$$

where λ is a variational parameter. to estimate the ground state energy. Compare the result with the exact answer.

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

$$E = -\frac{\hbar^2}{2m} \frac{\int_0^a dx \psi\psi''}{\int_0^a dx |\psi|^2} = -\frac{\hbar^2}{2m} \frac{A}{B}$$

where $' = d/dx$. We calculate A and B using $\psi' = -\lambda x^{\lambda-1}$:

$$A = \int_0^a dx \psi\psi'' = \int (\psi\psi')' - \int (\psi')^2 = 0 - \frac{\lambda^2 a^{2\lambda-1}}{2\lambda - 1}$$

$$B = \int_0^a dx \psi^2 = \int_0^a dx(a^{2\lambda} + x^{2\lambda} - 2a^\lambda x^\lambda) = a^{2\lambda+1}\left(1 + \frac{1}{2\lambda+1} - \frac{2}{\lambda+1}\right)$$
$$= \frac{2\lambda^2 a^{2\lambda+1}}{2\lambda^2 + 3\lambda + 1}$$

We then extremize E:

$$\frac{dE}{d\lambda} \propto \frac{Bd_\lambda A - Ad_\lambda B}{B^2}$$

where $d_\lambda = d/d\lambda$, gives

$$Bd_\lambda A - Ad_\lambda B = 0$$

Evaluating the derivatives using $d\lambda a^{p\lambda+q} = d\lambda e^{(p\lambda+q)\ln a} = (p\ln a)a^{p\lambda+q}$ 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

$$4\lambda^2 - 4\lambda - 5 = 0 \to \lambda = \frac{1+\sqrt{6}}{2}$$

This root give the best answer; also the negative root gives a sharp cusp at the origin. The ground state estimate becomes

$$E = -\frac{\hbar^2}{2m}\frac{A}{B} = -\frac{\hbar^2}{2m}\frac{2\lambda^2+3\lambda+1}{2(2\lambda-1)} \approx 2.4747\frac{\hbar^2}{2ma^2}$$

The exact solution is $\psi(x) = a^{-1/2}\cos(\pi x/2a)$ which gives

$$-\frac{\hbar^2}{2m}\psi'' = \frac{\hbar^2}{2m}\frac{\pi^2}{4a^2}\psi \to E = \frac{\pi^2}{4}\frac{\hbar^2}{2ma^2} \approx 2.4674\frac{\hbar^2}{2ma^2}$$

The agreement is very good and the variational estimate is greater than the ground state energy, as it must be.

8.9.45 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 $\hat{f}=\hat{\imath}+\hat{s}$ 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 $\vec{f}=\vec{\imath}+\vec{s}$ which is the total spin angular momentum. We note that

$$f^2=s^2+i^2+2\vec{s}\cdot\vec{\imath} \rightarrow \vec{s}\cdot\vec{\imath}=\frac{1}{2}(f^2-s^2-i^2)$$

This implies that the eigenstates of $\hat{H}_{HF}$ are coupled $\vec{s}$ and $\vec{\imath}$, i.e., $\{f^2, s^2, i^2, f_z\}$ or the good quantum numbers are

$$|n=1, \ell=0, s=1/2, \imath=1/2, f, m_f\rangle$$

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.

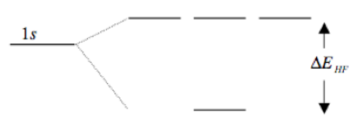


Figure 8.8: Hyperfine Splitting

Label all the quantum numbers for the four sublevels shown in the figure.

(d) Show that the energy level splitting is

$$\Delta E_{HF}=g_s g_i \mu_B \mu_N \langle\frac{1}{r^3}\rangle_{1s}$$

Show numerically that this splitting gives rise to the famous 21 cm radio frequency radiation used in astrophysical observations.

Using

$$\hat{f}^2\,|f m_f s i\rangle = f(f+1)\,|f m_f s i\rangle$$

$$\hat{s}^2 |fm_f si\rangle = s(s+1)|fm_f si\rangle = \frac{3}{4}|fm_f si\rangle$$

$$\hat{i}^2 |fm_f si\rangle = i(i+1)|fm_f si\rangle = \frac{3}{4}|fm_f si\rangle$$

we have

$$\vec{s}\cdot\vec{i}|fm_f si\rangle = \frac{1}{2}\left(f(f+1) - \frac{3}{2}\right)|fm_f si\rangle$$

so that

$$f = 0 \to \vec{s}\cdot\vec{i}|0,0,1/2,1/2\rangle = -\frac{3}{4}|0,0,1/2,1/2\rangle$$

$$f = 1 \to \vec{s}\cdot\vec{i}|1,m_f,1/2,1/2\rangle = +\frac{4}{4}|1,m_f,1/2,1/2\rangle$$

Therefore,

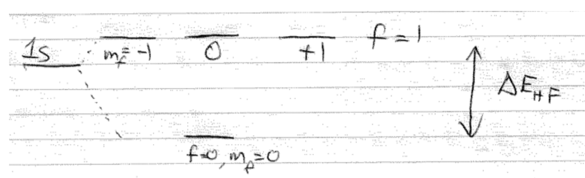
$$E_{1s(f=0)} = -\frac{3}{4}g_s g_i \mu_B \mu_N \left\langle \frac{1}{r^3}\right\rangle_{\ell s}$$

$$E_{1s(f=1)} = +\frac{1}{4}g_s g_i \mu_B \mu_N \left\langle \frac{1}{r^3}\right\rangle_{\ell s}$$

Thus,

$$\Delta E_{HF} = E_{1s(f=1)} - E_{1s(f=0)} = g_e g_p \mu_B \mu_N$$

The level diagram is



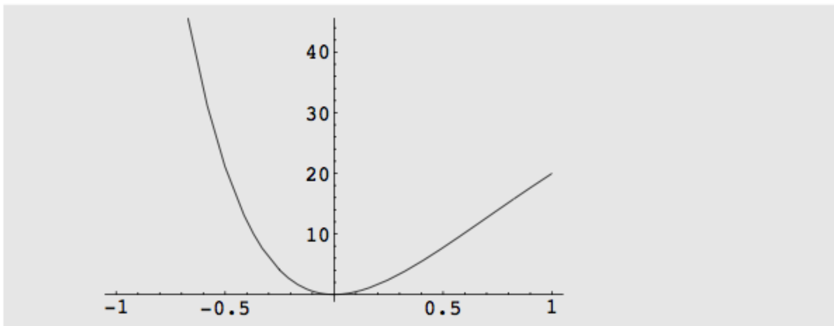
8.9.46 Find a Variational Trial Function

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:
If we try to identify the first term with the harmonic oscillator potential $m\omega^2 x^2$,

```
V = 50 (E^-x - 1)^2;
Plot[V, {x, -1, 1}];
```




```
Series[V, {x, 0, 3}]
```

$50\,x^2 - 50\,x^3 + O[x]^4$

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,

$$\psi1raw = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/4} E^{-m\,\omega\,x^2/(2\,\hbar)};$$

$$\psi1 = \psi1raw\ /.\ \{m \to 1,\ \omega \to 10,\ \hbar \to 1\}$$

$$e^{-5\,x^2}\left(\frac{10}{\pi}\right)^{1/4}$$

we compute the total energy using the Hamiltonian in the position space:

$$K1 = \frac{-\hbar^2}{2\,m}\ Integrate[\psi1\ D[\psi1, \{x, 2\}], \{x, -\infty, \infty\}]\ /.\ \{\hbar \to 1,\ m \to 1\}$$

$$\frac{5}{2}$$

$$P1 = Integrate[\psi1^2\ V, \{x, -\infty, \infty\}]$$

$$50\,(1 - 2\,e^{1/40} + e^{1/10})$$

$$Ebar1 = K1 + P1$$

$$\frac{5}{2} + 50\,(1 - 2\,e^{1/40} + e^{1/10})$$

```
N[Ebar1]
```

5.22703

The error is

$$\frac{\text{N[Ebar1]} - 39/8}{39/8}$$

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:

$$\psi 2 = \frac{1}{\pi^{1/4}\ \Delta^{1/2}}\ \text{E}^{-x^2/(2\Delta^2)};$$

$$\text{K2} = \frac{-\hbar^2}{2\ \text{m}}\ \text{Integrate}[\psi 2\ \text{D}[\psi 2,\ \{x,\ 2\}],\ \{x,\ -\infty,\ \infty\},\ \text{Assumptions} \to \Delta > 0]\ /.\ \{\hbar \to 1,\ \text{m} \to 1\}$$

$$\frac{1}{4\,\Delta^2}$$

$$\text{P2} = \text{Integrate}[\psi 2^2\ \text{V},\ \{x,\ -\infty,\ \infty\},\ \text{Assumptions} \to \Delta > 0]$$

$$50\left(1 - 2\,e^{\frac{\Delta^2}{4}} + e^{\Delta^2}\right)$$

$$\text{Ebar2} = \text{K2} + \text{P2}$$

$$50\left(1 - 2\,e^{\frac{\Delta^2}{4}} + e^{\Delta^2}\right) + \frac{1}{4\,\Delta^2}$$

$$\text{Ebar2min} = \text{FindMinimum}[\text{Ebar2},\ \{\Delta,\ 10^{-1/2}\}]$$

$$\{5.20891,\ \{\Delta \to 0.304036\}\}$$

$$\frac{\text{Ebar2min}[[1]] - 39/8}{39/8}$$

0.0684949

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

$$\psi 3 = (1 + k\,x)\,E^{-x^2/(2\Delta^2)};$$

It is not normalized at this point, and we calculate its norm

$$\text{norm2} = \text{Integrate}[\psi 3^2, \{x, -\infty, \infty\}, \text{Assumptions} \to \Delta > 0]$$

$$\frac{1}{2}\sqrt{\pi}\,\Delta\,(2 + k^2\,\Delta^2)$$

$$\text{K3} = \frac{-\hbar^2}{2\,m}\,\text{Integrate}[\psi 3\,D[\psi 3, \{x, 2\}], \{x, -\infty, \infty\}, \text{Assumptions} \to \Delta > 0]\ /.\ \{m \to 1, \hbar \to 1\}$$

$$\frac{\sqrt{\pi}\,(2 + 3\,k^2\,\Delta^2)}{8\,\Delta}$$

$$\text{P3} = \text{Integrate}[\psi 3^2\,V, \{x, -\infty, \infty\}, \text{Assumptions} \to \Delta > 0]$$

$$25\sqrt{\pi}\,\Delta\left(2 + k^2\,\Delta^2 + e^{\Delta^2}\,(2 + k\,\Delta^2\,(-4 + k + 2\,k\,\Delta^2)) - e^{\frac{\Delta^2}{4}}\,(4 + k\,\Delta^2\,(-4 + k\,(2 + \Delta^2)))\right)$$

$$\text{Ebar3} = \frac{\text{K3} + \text{P3}}{\text{norm2}}$$

$$\frac{1}{\sqrt{\pi}\,\Delta\,(2 + k^2\,\Delta^2)}\left(2\left(\frac{\sqrt{\pi}\,(2 + 3\,k^2\,\Delta^2)}{8\,\Delta} + 25\sqrt{\pi}\,\Delta\left(2 + k^2\,\Delta^2 + e^{\Delta^2}\,(2 + k\,\Delta^2\,(-4 + k + 2\,k\,\Delta^2)) - e^{\frac{\Delta^2}{4}}\,(4 + k\,\Delta^2\,(-4 + k\,(2 + \Delta^2)))\right)\right)\right)$$

$$\text{Ebar3min} = \text{FindMinimum}[\text{Ebar3}, \{\Delta, 10^{-1/2}\}, \{k, 0\}]$$

$$\{4.92615, \{\Delta \to 0.331205, k \to 0.764297\}\}$$

$$\frac{\text{Ebar3min}[[1]] - 39/8}{39/8}$$

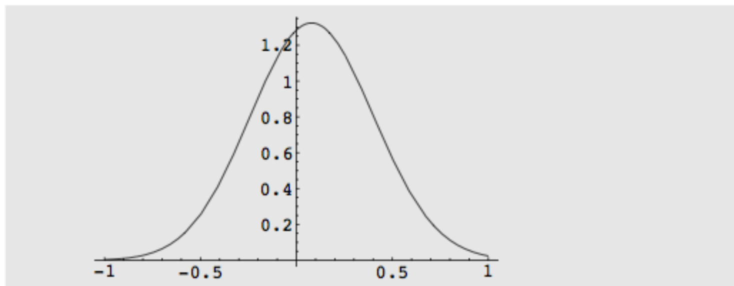
$$0.0104928$$

This is correct at the 1% level! The wave function is therefore

```
ψf = ψ3/Sqrt[norm2] /. Ebar3min[[2]]
```

$1.28474\, e^{-4.55801 x^2}\,(1 + 0.764297\, x)$

```
Plot[ψf, {x, -1, 1}];
```



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

```
Vm = D (E^(-a u) - 1)^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 it equilibrium distance $u = r - r_0$. The Schrodinger equation can be solved analytically. Expanding it around the minimum,

```
Series[Vm, {u, 0, 4}]
```

$a^2 D u^2 - a^3 D u^3 + \frac{7}{12} a^4 D u^4 + O[u]^5$

The harmonic oscillator approximation gives $\omega = \sqrt{2a^2 D/m}$. 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

```
ψm = E^(-d E^(-a u)) E^(-b a u/2);
```

where $b = 2d - 1$, $d = \sqrt{2Dm}/a\hbar$. Let us see that it satisfies the Schrodinger equation.

```
Simplify[(-ħ²/(2m) D[ψm, {u, 2}] + D (E^(-a u) - 1)^2 ψm)/ψm /. {b → 2 d - 1} /. {d -> Sqrt[2 D m]/(a ħ)}]
```

$$-\frac{a\hbar\left(-4\sqrt{2}\sqrt{Dm}+a\hbar\right)}{8m}$$

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

```
norm2m = Integrate[ψm^2, {u, -∞, ∞}, Assumptions → a > 0 && d > 0]
```

$$\frac{2^{-b}\, d^{-b}\, \mathrm{Gamma}[b]}{a}$$

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,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{du^2} + De^{-2au}\psi = 0$$

and change the variable to $y = e^{-au}$. 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

$$\psi \propto e^{-\sqrt{2mD}y/\hbar a}$$

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.

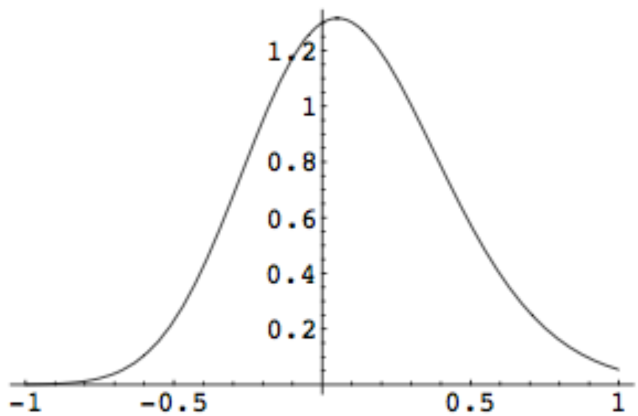
Back to the Morse potential. The case in this problem has $D = 50$, $a = 1$, $m = 1$, $\hbar = 1$. Therefore, the ground state energy is

$$E_0 = \frac{1}{2}\hbar a\sqrt{\frac{D}{2m}} - \frac{\hbar^2 a^2}{8m} = 5 - \frac{1}{8} = \frac{39}{8}$$

$$\psi mf = \text{Simplify}\left[\frac{1}{\sqrt{\text{norm2m}}}\,\psi m \;/.\; \{b \to 2\,d - 1\} \;/.\; \left\{d \to \frac{\sqrt{2\,D\,m}}{a\,\hbar}\right\} \;/.\; \{D \to 50,\ a \to 1,\ m \to 1,\ \hbar \to 1\}\right]$$

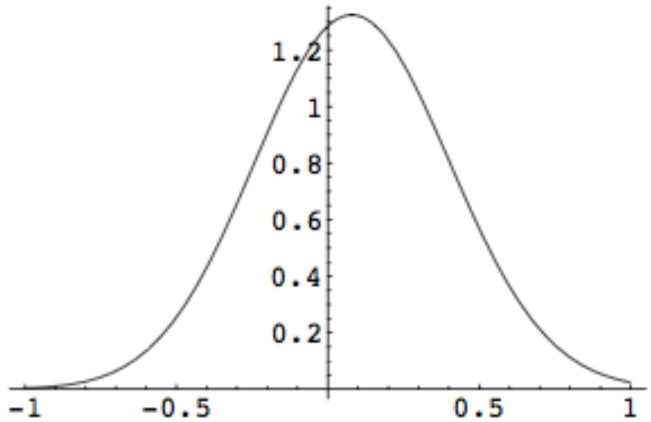
$$\frac{800000000\, e^{-10\, e^{-u} - \frac{19\, u}{2}}}{567\sqrt{2431}}$$

```
Plot[ψmf, {u, -1, 1}, PlotPoints → 50];
```

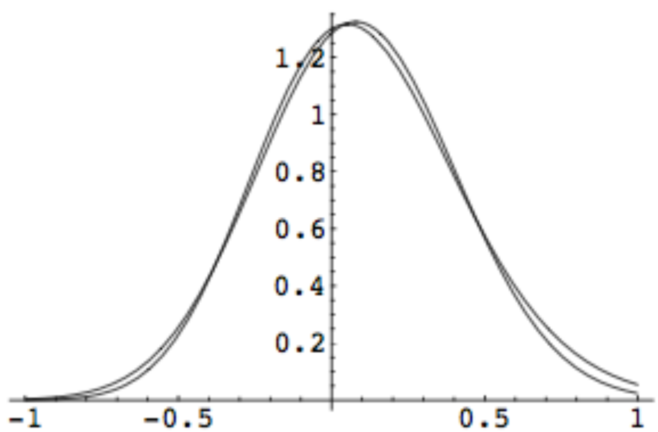


The variational linear time Gaussian wave function was

```
Plot[ψf, {x, -1, 1}, PlotPoints → 50];
```




```
Show[%, %%];
```



Quite close.

8.9.47 Hydrogen Corrections on 2s and 2p Levels

Work out the first-order shifts in energies of $2s$ and $2p$ states of the hydrogen atom due to relativistic corrections, the spin-orbit interaction and the so-called Darwin term,

$$-\frac{p^4}{8m_e^3c^2} + g\frac{1}{4m_e^2c^2}\frac{1}{r}\frac{dV_c}{dr}(\vec{L}\cdot\vec{S}) + \frac{\hbar^2}{8m_e^2c^2}\nabla^2 V_c \ , \ \ V_c = -\frac{Ze^2}{r}$$

where you should be able to show that $\nabla^2 V_c = 4\pi\delta(\vec{r})$. At the end of the calculation, take $g = 2$ and evaluate the energy shifts numerically.

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, $a = a_0/Z = \hbar^2/(Ze^2 m)$. Similarly,

$$R_{2p} = (2a)^{-3/2}\frac{r}{\sqrt{3}\,a} E^{-r/(2a)};$$

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

$$-\frac{\hbar^4}{8m^3c^2}\langle p^4\rangle = -\frac{1}{8m^3c^2}\langle(-\hbar^2\nabla^2)^2\rangle$$

$$\frac{1}{8m^3c^2}\int d^3x\psi^*\nabla^4\psi = -\frac{1}{8m^3c^2}\int d^3x(\nabla^2\psi)^*(\nabla^2\psi)$$

$$-\frac{1}{8m^3c^2}\int d^3x\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2}\right)(RY_\ell^m)^*\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2}\right)(RY_\ell^m)$$

$$-\frac{1}{8m^3c^2}\int r^2dr\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2}\right)R(r)\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2}\right)R(r)$$

The Darwin term for the Coulomb potential is proportional to

$$\Delta V_c = \nabla^2 \left(-\frac{Ze^2}{r} \right) = 4\pi Z e^2 \delta(\vec{x}) = 4\pi \frac{\hbar^2}{ma} \delta(\vec{x})$$

2s: First the relativistic correction

```
Integrate[-ħ^4/(8 m^3 c^2) (D[R2s, {r, 2}] + 2/r D[R2s, r])^2 r^2, {r, 0, ∞}, Assumptions → a > 0]
```

$$-\frac{13\,\hbar^4}{128\,a^4\,c^2\,m^3}$$

Second, the spin-orbit interaction. Because $L = 0$, it identically vanishes. Third, the Drawin term.

```
ħ^2/(8 m^2 c^2) 4 π ħ^2/(m a) ψ2s^2 /. {r → 0}
```

$$\frac{\hbar^4}{16\,a^4\,c^2\,m^3}$$

```
% + %%
```

$$-\frac{5\,\hbar^4}{128\,a^4\,c^2\,m^3}$$

2p$_{1/2}$: For the relativistic correction

```
Integrate[-ħ^4/(8 m^3 c^2) (D[R2p, {r, 2}] + 2/r D[R2p, r] - 2/r^2 R2p)^2 r^2,
  {r, 0, ∞}, Assumptions → a > 0]
```

$$-\frac{7\,\hbar^4}{384\,a^4\,c^2\,m^3}$$

Second, the spin-orbit interaction.

```
Integrate[g/(4 m^2 c^2) 1/r^3 ħ^2/(m a) (-ħ^2) R2p^2 r^2, {r, 0, ∞}, Assumptions → a > 0]
```

$$-\frac{g\,\hbar^4}{96\,a^4\,c^2\,m^3}$$

Third, the Darwin term. Because the wave function vanishes at the origin, it is identically zero.

```
% + %% /. {g → 2}
```

$$-\frac{5\,\hbar^4}{128\,a^4\,c^2\,m^3}$$

2p$_{3/2}$: First, the relativistic correction. We use the fact that

$$p^2\psi = -\hbar^2 Y_1^m \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{2}{r^2}\right) R(r)$$

```
Integrate[-ℏ^4/(8 m^3 c^2) (D[R2p, {r, 2}] + 2/r D[R2p, r] - 2/r^2 R2p)^2 r^2,
 {r, 0, ∞}, Assumptions → a > 0]
```

$$-\frac{7\,\hbar^4}{384\,a^4\,c^2\,m^3}$$

Second, the spin-orbit interaction.

```
Integrate[g/(4 m^2 c^2) 1/r^3 ℏ^2/(m a) ℏ^2/2 R2p^2 r^2, {r, 0, ∞}, Assumptions → a > 0]
```

$$\frac{g\,\hbar^4}{192\,a^4\,c^2\,m^3}$$

Third, the Darwin term. Because the wave function vanishes at the origin, it is identically zero.

```
% + %% /. {g → 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

$$-\frac{e^2}{8a} - \frac{5\hbar^4}{128a^4m^3c^2} = -\frac{e^2}{a}\left(\frac{1}{8} + \frac{5}{128}\alpha^2\right)$$

while the $2p_{3/2}$ states have the energy

$$-\frac{e^2}{a}\left(\frac{1}{8}+\frac{1}{128}\alpha^2\right)$$

where $a = e^3/\hbar c$. Numerically,(we took $g = 2$ above for comparison between $2s$ and $2p$), the energy shifts in eV are

```
constants =
  {e → 1.60217653 * 10^-19 * 2.997925 * 10^9 , a -> 5.291772108 * 10^-9 , α -> 1 / 137.03599911};
ergtoev = 6.241506 * 10^11 ;
(-e^2/a (5/128 α^2) /. constants) * ergtoev
(-e^2/a (1/128 α^2) /. constants) * ergtoev
% - %%
```

```
-0.0000566032
```

```
-0.0000113206
```

```
0.0000452826
```

8.9.48 Hyperfine Interaction Again

Show that the interaction between two magnetic moments is given by the Hamiltonian

$$H = -\frac{2}{3}\mu_0(\vec{\mu}_1 \cdot \vec{\mu}_2)\delta(\vec{x}-\vec{y}) - \frac{\mu_0}{4\pi}\frac{1}{r^3}\left(3\frac{r_i r_j}{r^2} - \delta_{ij}\right)\mu_1^i \mu_2^j$$

where $r_i = x_i - y_i$. (NOTE: Einstein summation convention used above). Use first-order perturbation to calculate the splitting between $F = 0, 1$ levels of the hydrogen atoms and the corresponding wavelength of the photon emission. How does the splitting compare to the temperature of the cosmic microwave background?

We start with Maxwell's equations

$$\begin{aligned}
\nabla \cdot \vec{E} &= 4\pi\rho \\
\nabla \times \vec{B} &= \frac{1}{c}\dot{\vec{E}} + \frac{4\pi}{c}\vec{j} \\
\nabla \times \vec{E} &= -\frac{1}{c}\dot{\vec{B}} \\
\nabla \cdot \vec{B} &= 0
\end{aligned}$$

They are derived from the action

$$S = \int dt\, d^3x \left(\frac{1}{8\pi}(E^2 + B^2) - \phi\rho + \frac{1}{c}\vec{A}\cdot\vec{j} \right)$$

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

$$\vec{B} = \frac{8\pi}{3}\vec{\mu}\delta(\vec{x}-\vec{y}) + \frac{1}{r^3}\left(3\frac{\vec{r}}{r}\frac{\vec{\mu}\cdot\vec{r}}{r} - \vec{\mu}\right)$$

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 $\vec{y}$

$$H = -\vec{\mu}_1 \cdot \vec{B}(\vec{x}) = -\frac{8\pi}{3}\vec{\mu}_1 \cdot \vec{\mu}_2\delta(\vec{x}-\vec{y}) - \frac{1}{r^3}\left(3\frac{\vec{\mu}_1\cdot\vec{r}}{r}\frac{\vec{\mu}_2\cdot\vec{r}}{r} - \vec{\mu}_1\cdot\vec{\mu}_2\right)$$

In the MKSA system, it is

$$H = -\vec{\mu}_1 \cdot \vec{B}(\vec{x}) = -\frac{2\mu_0}{3}\vec{\mu}_1 \cdot \vec{\mu}_2\delta(\vec{x}-\vec{y}) - \frac{\mu_0}{4\pi r^3}\left(3\frac{\vec{\mu}_1\cdot\vec{r}}{r}\frac{\vec{\mu}_2\cdot\vec{r}}{r} - \vec{\mu}_1\cdot\vec{\mu}_2\right)$$

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

$$H = +\frac{2\mu_0}{3}2.79\mu_N\mu_e\frac{4}{\hbar^2}(\vec{s}_p\cdot\vec{s}_e)\delta(\vec{x})$$

The first order perturbation of this Hamiltonian gives the hyperfine splitting

$$E_{ff} = +\frac{2\mu_0}{3}2.79\mu_N\mu_e\frac{4}{\hbar^2}(\vec{s}_p\cdot\vec{s}_e)|\psi(0)|^2$$

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

$$\begin{aligned}\Delta E &= \frac{2\mu_0}{3} 2.79 \mu_N \mu_e \frac{4}{\hbar^2} \left(\frac{\hbar^2}{4} - \left(-\frac{3\hbar^2}{4} \right) \right) \\ &= \frac{2\mu_0}{3} 2.79 \mu_N \mu_e \frac{4}{\pi a_0^3} = 9.39 \times 10^{-25}\, J\end{aligned}$$

Parametrically, it is $\alpha^2 (m_e/m_p)$ times the binding energy and hence even more suppressed than the fine structure.

The cosmic thermal bath has $T = 2.7^\circ\, K$ and hence $kT = 3.7 \times 10^{-23}\, J$, 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 21cm line*. It has had an important impact on astronomy. Because the wavelength is much longer than typical dust particles, it can bee 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.

8.9.49 A Perturbation Example

Suppose we have two spin$-1/2$ degrees of freedom, A and B. Let the initial Hamiltonian for this joint system be given by

$$H_0 = -\gamma B_z \left(S_z^A \otimes I^B + I^A \otimes S_z^B \right)$$

where I^A and I^B are identity operators, S_z^A is the observable for the $z-$component of the spin for the system A, and S_z^B is the observable for the $z-$component of the spin for the system B. Here the notation is meant to emphasize that both spins experience the same magnetic field $\vec{B} = B_z \hat{z}$ and have the same gyromagnetic ratio γ.

(a) Determine the energy eigenvalues and eigenstates for H_0

It is easy to intuit,

$$\begin{aligned} &\left|+_z\right\rangle_A \otimes \left|+_z\right\rangle_B \quad E_{++} = \hbar\omega_L \\ &\left|+_z\right\rangle_A \otimes \left|-_z\right\rangle_B \quad E_{+-} = 0 \\ &\left|-_z\right\rangle_A \otimes \left|+_z\right\rangle_B \quad E_{-+} = 0 \\ &\left|-_z\right\rangle_A \otimes \left|-_z\right\rangle_B \quad E_{--} = -\hbar\omega_L \end{aligned}$$

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 $H_{total} = H_0 + W$, 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:

$$E_{++} \to E_{++} + \langle ++| W |++\rangle = \hbar\omega_L + \lambda \frac{hbar^2}{4}$$
$$E_{--} \to E_{--} + \langle --| W |--\rangle = -\hbar\omega_L + \lambda \frac{hbar^2}{4}$$

For E_{+-} and E_{-+}, we need to diagonalize the restriction of W on the corresponding subspace. The matrix representation of this restriction is

$$W_0 \leftrightarrow \begin{pmatrix} \langle +-| W |+-\rangle & \langle +-| W |-+\rangle \\ \langle -+| W |+-\rangle & \langle -+| W |-+\rangle \end{pmatrix}$$

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,

$$S_x^A \otimes S_x^B \leftrightarrow \frac{\hbar^2}{4} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad , \quad S_y^A \otimes S_y^B \leftrightarrow \frac{\hbar^2}{4} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$S_z^A \otimes S_z^B \leftrightarrow \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad , \quad W \leftrightarrow \lambda \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

With the corresponding vector representations of $|+-\rangle$ and $|-+\rangle$,

$$|+-\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad , \quad |-+\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

we have

$$\langle +-| W |-+\rangle = \lambda \frac{\hbar^2}{2} \quad , \quad \langle -+| W |+-\rangle = \lambda \frac{\hbar^2}{2}$$
$$\langle +-| W |+-\rangle = \lambda - \frac{\hbar^2}{2} \quad , \quad \langle -+| W |-+\rangle = -\lambda \frac{\hbar^2}{2}$$

So in the end

$$W_0 \leftrightarrow \lambda \frac{\hbar^2}{4} \begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix}$$

The eigenvalue equation is

$$(-1-\epsilon)^2 - 4 = 0 \rightarrow \epsilon + 1 = \pm 2$$

so

$$\epsilon = \left\{ \lambda\frac{\hbar^2}{4}, -3\lambda\frac{\hbar^2}{4} \right\}$$

and the corresponding eigenvectors are determined by

$$\begin{pmatrix} -2 & 2 \\ 2 & -2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0 \rightarrow \begin{pmatrix} a \\ b \end{pmatrix} \propto \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0 \rightarrow \begin{pmatrix} a \\ b \end{pmatrix} \propto \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and so the proper zeroth-order states in the degenerate subspace for H_0 are

$$|W_+\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) \quad , \quad |W_-\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$$

with corresponding energy corrections

$$\langle W_+| \, W_0 \, |W_+\rangle = \lambda\frac{\hbar^2}{4} \quad , \quad \langle W_-| \, W_0 \, |W_-\rangle = -3\lambda\frac{\hbar^2}{4}$$

Finally, the first-order energy corrections are

$$\{\hbar\omega_L, 0, 0, -\hbar\omega_L\} \rightarrow \left\{ \hbar\omega_L + \lambda\frac{\hbar^2}{4}, \lambda\frac{\hbar^2}{4}, -3\lambda\frac{\hbar^2}{4}, -\hbar\omega_L - 3\lambda\frac{\hbar^2}{4} \right\}$$

8.9.50 More Perturbation Practice

Consider two spi$-1/2$ degrees of freedom, whose joint pure states can be represented by state vectors in the tensor-product Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$, where $\mathcal{H}_A$ and $\mathcal{H}_B$ are each two-dimensional. Suppose that the initial Hamiltonian for the spins is

$$H_0 = \left(-\gamma_A B_z S_z^A\right) \otimes I^B + I^A \otimes \left(-\gamma_B B_z S_z^B\right)$$

(a) Compute the eigenstates and eigenenergies of H_0, assuming $\gamma_A \neq \gamma_B$ and that the gyromagnetic ratios are non-zero. If it is obvious to you what the eigenstates are, you can just guess them and compute the eigenenergies.

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

$$W = \alpha S_x^A \otimes S_x^B$$

where α 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

$$S_x^A \otimes S_x^B |+_a +_b\rangle = \frac{\hbar^2}{4} |-_a -_b\rangle$$
$$S_x^A \otimes S_x^B |+_a -_b\rangle = \frac{\hbar^2}{4} |-_a +_b\rangle$$
$$S_x^A \otimes S_x^B |-_a +_b\rangle = \frac{\hbar^2}{4} |+_a -_b\rangle$$
$$S_x^A \otimes S_x^B |-_a -_b\rangle = \frac{\hbar^2}{4} |+_a +_b\rangle$$

For the $|+_a +_b\rangle$ state,

$$\lambda |1\rangle \rightarrow -\frac{\hbar^2}{4} \frac{\langle -_a -_b | W |+_a +_b\rangle}{\hbar(\gamma_a + \gamma_b)B_z} = -\frac{\hbar\alpha}{4(\gamma_a + \gamma_b)B_z} |-_a -_b\rangle$$

Similarly, for the $|+_a -_b\rangle$ state

$$\lambda |1\rangle \rightarrow -\frac{\hbar^2}{4} \frac{\langle -_a +_b | W |+_a -_b\rangle}{\hbar(-\gamma_a + \gamma_b)B_z} = -\frac{\hbar\alpha}{4(\gamma_a - \gamma_b)B_z} |-_a +_b\rangle$$

For the $|-_a +_b\rangle$ state,

$$\lambda |1\rangle \rightarrow -\frac{\hbar^2}{4} \frac{\langle +_a -_b | W |-_a +_b\rangle}{\hbar(\gamma_a - \gamma_b)B_z} = \frac{\hbar\alpha}{4(\gamma_a - \gamma_b)B_z} |+_a -_b\rangle$$

and for the $|-_a -_b\rangle$ state,

$$\lambda |1\rangle \rightarrow -\frac{\hbar^2}{4} \frac{\langle +_a +_b | W |-_a -_b\rangle}{\hbar(\gamma_a + \gamma_b)B_z} = \frac{\hbar\alpha}{4(\gamma_a + \gamma_b)B_z} |+_a +_b\rangle$$

Chapter 9

Time-Dependent Perturbation Theory

9.5 Problems

9.5.1 Square Well Perturbed by an Electric Field

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

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

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

In the $n = 1$ state of this potential well, the electron has these wave functions and corresponding energies

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n}{a}\left(\frac{a}{2} + x\right)\right) \quad , \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$$

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

$$H'_{n_1 n_2} = \langle n_1 | H' | n_2 \rangle = \frac{e\varepsilon}{a} \int_{-a/2}^{a/2} \sin\left(\frac{\pi n_1}{a}\left(\frac{a}{2}+x\right)\right) \sin\left(\frac{\pi n_2}{a}\left(\frac{a}{2}+x\right)\right) x dx$$

$$= \frac{e\varepsilon}{a} \int_{-a/2}^{a/2} \left[\cos\left(\frac{\pi(n_1-n_2)}{a}\left(\frac{a}{2}+x\right)\right) - \cos\left(\frac{\pi(n_1+n_2)}{a}\left(\frac{a}{2}+x\right)\right)\right] x dx$$

$$= \frac{e\varepsilon}{a}\left[\frac{a^2}{(n_1-n_2)^2\pi^2}\left((-1)^{n_1-n_2}-1\right) - \frac{a^2}{(n_1+n_2)^2\pi^2}\left((-1)^{n_1+n_2}-1\right)\right]$$

$$= \frac{4e\varepsilon a}{\pi^2} \frac{n_1 n_2}{(n_1^2-n_2^2)^2}\left((-1)^{n_1+n_2}-1\right)$$

since

$$\left((-1)^{n_1+n_2}-1\right) = \left((-1)^{n_1-n_2}-1\right)$$

for all n_1, n_2. We also define

$$\omega_{n_1 n_2} = \frac{E_{n_2}-E_{n_1}}{\hbar} = \frac{\hbar\pi^2}{2ma^2}(n_2^2-n_1^2)$$

Now, in time-dependent perturbation theory the amplitude for the transition $q \to p$ is given by

$$C_{pq}(t) = \frac{1}{i\hbar}\int_0^\tau H'_{pq} e^{i\omega_{pq}t} dt = \frac{1}{\hbar\omega_{pq}} H'_{pq}\left(1-e^{i\omega_{pq}\tau}\right)$$

when H'_{pq} is time-independent. For the transition $1 \to 2$ we have

$$H'_{21} = \frac{4e\varepsilon a}{\pi^2}\frac{2}{9}(-2) = -\frac{16e\varepsilon a}{9\pi^2} \quad , \quad \omega_{21} = \frac{3\hbar\pi^2}{2ma^2}$$

so that the probability finding the electron in the $n=2$ state at $t > \tau$ is

$$P_2(t>\tau) = |C_{21}(t)|^2 = \frac{1}{\hbar^2\omega_{21}^2} H_{21}^{'2}\left(1-e^{i\omega_{pq}\tau}\right)\left(1-e^{-i\omega_{pq}\tau}\right)$$

$$= \frac{1}{\hbar^2\left(\frac{3\hbar\pi^2}{2ma^2}\right)^2}\left(-\frac{16e\varepsilon a}{9\pi^2}\right)^2 (2-2\cos\frac{3\hbar\pi^2}{2ma^2}\tau)$$

$$= \frac{4m^2a^4}{9\hbar^4\pi^4}\frac{256e^2\varepsilon^2a^2}{81\pi^2} 4\sin^2\frac{3\hbar\pi^2}{4ma^2}\tau = \frac{4^6 m^2 a^6 e^2 \varepsilon^2}{3^6\hbar^4\pi^6}\sin^2\frac{3\hbar\pi^2}{4ma^2}\tau$$

For small τ

$$P_2(t>\tau) = \frac{4^6 m^2 a^6 e^2 \varepsilon^2}{3^6\hbar^4\pi^6}\left(\frac{3\hbar\pi^2}{4ma^2}\tau\right)^2 = \frac{4^4 a^2 e^2 \varepsilon^2}{3^4\hbar^2\pi^2}\tau^2$$

For the transition $1 \to 3$ we have

$$H'_{31} = 0 \to P_3(t>\tau) = |C_{31}(t)|^2 = 0$$

9.5.2 3-Dimensional Oscillator in an electric field

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

$$V(x,y,z) = k\left(x^2+y^2+z^2\right) \tag{9.-8}$$

(a) Find the three lowest energy levels E_0, E_1, E_2 and their associated degeneracy.

Using Cartesian coordinates

$$\begin{array}{l} E_N = E_n + E_\ell + E_m = \frac{3}{2}\hbar\omega + (n+\ell+m)\hbar\omega = \frac{3}{2}\hbar\omega + N\hbar\omega \\ N = n+\ell+m = 0,1,2,...... \quad , \quad \omega = \sqrt{\frac{2k}{M}} \end{array}$$

Therefore,

$$\begin{array}{l} E_0 = \frac{3}{2}\hbar\omega = \frac{3}{2}\hbar\sqrt{\frac{2k}{M}} \to \text{non}-\text{degenerate} \quad \psi_{000} \\ E_1 = \frac{5}{2}\hbar\omega = \frac{5}{2}\hbar\sqrt{\frac{2k}{M}} \to 3-\text{folddegenerate} \quad \psi_{100},\psi_{010},\psi_{001} \\ E_2 = \frac{7}{2}\hbar\omega = \frac{7}{2}\hbar\sqrt{\frac{2k}{M}} \to 6-\text{folddegenerate} \quad \psi_{200},\psi_{020},\psi_{002},\psi_{110},\psi_{101},\psi_{011} \\ \text{degeneracy} = f_N = \frac{1}{2}(N+1)(N+2) \end{array}$$

(b) Suppose a small perturbing potential $Ax\cos\bar{\omega}t$ causes transitions among the various states in (a). Using a convenient basis for degenerate states, specify in detail the allowed transitions neglecting effects proportional to A^2 or higher.

At time $t=0$, $H' = Ax\cos\bar{\omega}t$. The first order perturbation correction gives with ℓ being the quantum number for the component oscillator along the $x-$axis

$$\begin{aligned} \langle \ell' m' n'| H'(x,t) |\ell m n\rangle &= \delta_{m'm}\delta_{n'n}\langle \ell'| H'(x,t) |\ell\rangle = A\cos\bar{\omega}t\delta_{m'm}\delta_{n'n}\langle \ell'| x |\ell\rangle \\ &= A\alpha\cos\bar{\omega}t\delta_{m'm}\delta_{n'n}\left[\sqrt{\ell+1}\delta_{\ell',\ell+1} + \sqrt{\ell}\delta_{\ell',\ell-1}\right] \end{aligned}$$

where

$$\alpha = \sqrt{\frac{\hbar}{2M\omega}} = \sqrt{\frac{\hbar}{2M\sqrt{\frac{2k}{M}}}} = \left(\frac{h^2}{2kM}\right)^{1/4}$$

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.

Between the states corresponding to energies E_0 and E_1, the selection rules allow only the transition $\psi_{000} \to \psi_{100}$. The corresponding probability is

$$P_{10} = \frac{1}{\hbar^2}\left|\int_0^t H'_{10}e^{i\omega t}dt\right|^2 = \frac{A^2\alpha^2}{\hbar^2}\left|\int_0^t \cos\bar{\omega}te^{i\omega t}dt\right|^2$$

where we have used

$$H'_{10} = \langle 100|\, H'(x,t)\,|000\rangle = A\alpha\cos\omega t$$

Now,

$$\int_0^t \cos\bar{\omega}te^{i\omega t}dt = \frac{1}{2i}\left[\frac{e^{i(\omega+\bar{\omega})t}-1}{\omega+\bar{\omega}} + \frac{e^{i(\omega-\bar{\omega})t}-1}{\omega-\bar{\omega}}\right]$$

In the microscopic world, ω and $\bar{\omega}$ are usually very large. Thus, only for $\omega \approx \bar{\omega}$, will the above integral be large. Thus,

$$P_{10} \approx \frac{A^2\alpha^2}{\hbar^2}\frac{\sin^2\left((\omega-\bar{\omega})t/2\right)}{\left((\omega-\bar{\omega})/2\right)^2}$$

or when t gets *large enough*

$$\frac{\sin^2\left((\omega-\bar{\omega})t/2\right)}{\left((\omega-\bar{\omega})/2\right)^2} \to 2\pi t\delta(\omega-\bar{\omega})$$

so that

$$P_{10} \approx \frac{2\pi A^2\alpha^2 t}{\hbar^2}\delta(\omega-\bar{\omega})$$

and the transition rate is

$$\frac{P_{10}}{t} \approx \frac{2\pi A^2\alpha^2}{\hbar^2}\delta(\omega-\bar{\omega})$$

9.5.3 Hydrogen in decaying potential

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

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

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

To $1^{st}-$order the $1s \to 2s$ 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

$1s \to 2p$ ($\Delta\ell = +1$) transition is allowed in first order and we must also have $\Delta m = 0$.

With the potential energy

$$V = -e\mathcal{E}_0 z e^{-t/\tau}$$

for $t > 0$, we have the only non-vanishing first-order transition amplitude

$$\begin{aligned} c^{(1)}(t) &= -\left(-\frac{i}{\hbar}\right) e\mathcal{E}_0 \int_0^t dt \left\langle 210\right| z \left|100\right\rangle e^{(i\omega - 1/\tau)t} \\ &= \frac{ie\mathcal{E}_0}{\hbar} \left\langle 210\right| z \left|100\right\rangle \frac{\left(e^{(i\omega-1/\tau)t} - 1\right)}{\omega^2 + \frac{1}{\tau^2}} (-i\omega - 1/\tau) \end{aligned}$$

The probability is then

$$P = \left|c^{(1)}(t)\right|^2 = \left(\frac{e\mathcal{E}_0}{\hbar}\right)^2 \frac{1}{\omega^2 + \frac{1}{\tau^2}} \left|\left\langle 210\right| z \left|100\right\rangle\right|^2 \left(1 + e^{-2t/\tau} - 2e^{-t/\tau}\cos\omega t\right)$$

For $t \gg \tau$ ($t \to \infty$ essentially) we have

$$P = \left(\frac{e\mathcal{E}_0}{\hbar}\right)^2 \frac{1}{\omega^2 + \frac{1}{\tau^2}} \left|\left\langle 210\right| z \left|100\right\rangle\right|^2$$

Now,

$$\left\langle 210\right| z \left|100\right\rangle = 2\pi \int_{-1}^{1} d(\cos\theta) \int_0^\infty r^2 dr R_{21} Y_{10} r \cos\theta R_{10} Y_{00} = \frac{2^{15/2}}{3^5} a_0$$

Therefore,

$$P = \left(\frac{e\mathcal{E}_0}{\hbar}\right)^2 \frac{a_0^2}{\omega^2 + \frac{1}{\tau^2}} \frac{2^{15}}{3^{10}}$$

where

$$\omega = \frac{E_{2p} - E_{1s}}{\hbar} = \frac{3e^2}{8a_0\hbar}$$

9.5.4 2 spins in a time-dependent potential

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

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

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

(a) by solving the problem exactly.

We have (using the $|S, S_z\rangle$ basis)

$$\hat{H} = \left(\frac{4\Delta}{\hbar^2}\right)\hat{S}_1 \cdot \hat{S}_2 = 4\Delta\left(\frac{\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2}{2\hbar^2}\right) \to 4\Delta\left(\frac{S(S+1) - 3/2}{2}\right) = \begin{cases} \Delta & S = 1 \\ -3\Delta & S = 0 \end{cases}$$

so that

$$\hat{H}\,|1, M\rangle = \Delta\,|1, M\rangle \quad , \quad \hat{H}\,|0, 0\rangle = -3\Delta\,|0, 0\rangle$$

We get the exact solution as follows: At $t = 0$,

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

At later t,

$$\begin{aligned} |\psi(t)\rangle &= \frac{1}{\sqrt{2}}\left(e^{-i\Delta t/\hbar}\,|1, 0\rangle + e^{-i3\Delta t/\hbar}\,|0, 0\rangle\right) \\ &= \frac{1}{2}\left(e^{-i\Delta t/\hbar}\left(|+-\rangle + |-+\rangle\right) + e^{-i3\Delta t/\hbar}\left(|+-\rangle - |-+\rangle\right)\right) \\ &= \frac{1}{2}\left(\left(e^{-i\Delta t/\hbar} + e^{-i3\Delta t/\hbar}\right)|+-\rangle + \left(e^{-i\Delta t/\hbar} - e^{-i3\Delta t/\hbar}\right)|-+\rangle\right) \end{aligned}$$

Therefore,

$$\begin{aligned} P_{+-}(t) &= \left|\langle +- \mid \psi(t)\rangle\right|^2 = \tfrac{1}{4}\left|e^{-i\Delta t/\hbar} + e^{-i3\Delta t/\hbar}\right|^2 = \tfrac{1}{2} + \tfrac{1}{2}\cos\tfrac{4\Delta t}{\hbar} \\ P_{-+}(t) &= \left|\langle -+ \mid \psi(t)\rangle\right|^2 = \tfrac{1}{4}\left|e^{-i\Delta t/\hbar} - e^{-i3\Delta t/\hbar}\right|^2 = \tfrac{1}{2} - \tfrac{1}{2}\cos\tfrac{4\Delta t}{\hbar} \\ P_{++}(t) &= \left|\langle ++ \mid \psi(t)\rangle\right|^2 = 0 = \left|\langle -- \mid \psi(t)\rangle\right|^2 = P_{--}(t) \end{aligned}$$

(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

$$c_{+-}^{(1)} = -\frac{i}{\hbar}\int_0^t \langle +-|\hat{H}\,|+-\rangle\,dt \quad , \quad c_{-+}^{(1)} = -\frac{i}{\hbar}\int_0^t \langle -+|\hat{H}\,|+-\rangle\,dt$$

Now using,

$$|+-\rangle = \frac{1}{\sqrt{2}}\left(|1, 0\rangle + |0, 0\rangle\right) \quad , \quad |-+\rangle = \frac{1}{\sqrt{2}}\left(|1, 0\rangle - |0, 0\rangle\right)$$

we have

$$c_{+-}^{(1)} = -\frac{i\Delta t}{\hbar}\left(\frac{1-3}{2}\right) = \frac{i\Delta t}{\hbar} \quad , \quad c_{-+}^{(1)} = -\frac{i\Delta t}{\hbar}\left(\frac{1+3}{2}\right) = -\frac{2i\Delta t}{\hbar}$$

In addition, $c_{++}^{(1)} = c_{--}^{(1)} = 0$ because $\hat{H}$ only connects states of the same $M_{total} = m_1 + m_2$, which is zero for this initial state.

Therefore, we have

$$\begin{aligned} P_{+-}(t) &= |c_{+-}(t)|^2 = \left|1 + \tfrac{i\Delta t}{\hbar}\right|^2 = 1 + \tfrac{\Delta^2 t^2}{\hbar^2} \\ P_{-+}(t) &= |c_{-+}(t)|^2 = \left|-\tfrac{2i\Delta t}{\hbar}\right|^2 = \tfrac{4\Delta^2 t^2}{\hbar^2} \\ P_{++}(t) &= |c_{++}(t)|^2 = 0 = |c_{--}(t)|^2 = P_{--}(t) \end{aligned}$$

We note that the exact solutions expanded to first order are

$$P_{-+}(t) = \frac{1}{2} - \frac{1}{2}\cos\frac{4\Delta t}{\hbar} = \frac{1}{2} - \frac{1}{2}\left(1 - \frac{1}{2}\left(\frac{4\Delta t}{\hbar}\right)^2\right) = \frac{4\Delta^2 t^2}{\hbar^2}$$

in agreement with perturbation theory, but

$$P_{+-}(t) = \frac{1}{2} + \frac{1}{2}\cos\frac{4\Delta t}{\hbar} = \frac{1}{2} + \frac{1}{2}\left(1 - \frac{1}{2}\left(\frac{4\Delta t}{\hbar}\right)^2\right) = 1 - \frac{4\Delta^2 t^2}{\hbar^2}$$

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 $t >> \hbar/\Delta$ since the lowest order expression gives a poor approximation to the exact answer.

9.5.5 A Variational Calculation of the Deuteron Ground State Energy

Use the empirical potential energy function

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

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

Try a simple variational function of the form

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

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

We have

$$V(r) = -Ae^{-r/a}\ ,\ A = 32.7\,MeV,\ a = 2.18 \times 10^{-13} cm$$

We also assume that $\ell = 0$. Then

$$E_0 \leq \frac{\langle\psi|\,\hat{H}\,|\psi\rangle}{\langle\psi\mid\psi\rangle}$$

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 $\ell = 0$)

$$\begin{aligned}\nabla^2\psi(r) &= \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{de^{-\alpha r/2a}}{dr}\right) = \frac{1}{r^2}\frac{d}{dr}\left(-\frac{\alpha}{2a}r^2 e^{-\alpha r/2a}\right)\\ &= -\frac{\alpha}{2a}\left(\frac{2}{r} - \frac{\alpha}{2a}\right)e^{-\alpha r/2a} = \left(-\frac{\alpha}{a}\frac{1}{r} + \left(\frac{\alpha}{2a}\right)^2\right)e^{-\alpha r/2a}\end{aligned}$$

Therefore,

$$\begin{aligned}\langle\psi|\,\hat{H}\,|\psi\rangle &= 4\pi\int_0^\infty r^2 dr e^{-\alpha r/a}\left(-\frac{\hbar^2}{2m_D}\left(-\frac{\alpha}{a}\frac{1}{r} + \left(\frac{\alpha}{2a}\right)^2\right) - Ae^{-r/a}\right)\\ &= 4\pi\left[\frac{\hbar^2}{2m_D}\frac{\alpha}{a}\int_0^\infty r dr e^{-\alpha r/a} - \frac{\hbar^2}{2m_D}\left(\frac{\alpha}{2a}\right)^2\int_0^\infty r^2 dr e^{-\alpha r/a} - A\int_0^\infty r^2 dr e^{-(1+\alpha)r/a}\right]\\ &= 4\pi\left[\frac{\hbar^2}{2m_D}\frac{\alpha}{a}\frac{1}{\left(\frac{\alpha}{a}\right)^2} - \frac{\hbar^2}{2m_D}\left(\frac{\alpha}{2a}\right)^2\frac{2}{\left(\frac{\alpha}{a}\right)^3} - A\frac{2}{\left(\frac{1+\alpha}{a}\right)^3}\right]\\ &= 4\pi\left[\frac{\hbar^2}{4m_D}\frac{a}{\alpha} - 2A\frac{a^3}{(1+\alpha)^3}\right]\end{aligned}$$

and

$$\langle\psi \mid \psi\rangle = 4\pi \int_0^\infty r^2 dr e^{-\alpha r/a} = 4\pi \frac{2}{\left(\frac{\alpha}{a}\right)^3} = 8\pi \left(\frac{a}{\alpha}\right)^3$$

where we have used

$$\int_0^\infty x^n e^{-\rho x} dx = \frac{n!}{\rho^{n+1}}$$

Thus,

$$E_0 \leq \frac{4\pi \left[\frac{\hbar^2}{4m_D}\frac{a}{\alpha} - 2A\frac{a^3}{(1+\alpha)^3}\right]}{8\pi \left(\frac{a}{\alpha}\right)^3} = \frac{1}{2}\frac{\alpha^2}{a^2}\left(\frac{\hbar^2}{4m_D} - 2A\frac{a^2\alpha}{(1+\alpha)^3}\right)$$

One solution is $\alpha = 0 \to E_0 \leq 0$, which we already know is true; so we ignore this solution. The second solution is given by

$$\begin{aligned}
&0 = \left(\tfrac{\hbar^2}{4m_D} - 2A\tfrac{a^2\alpha}{(1+\alpha)^3}\right) + \alpha\left(-A\tfrac{a^3}{(1+\alpha)^3} + 3A\tfrac{a^2\alpha}{(1+\alpha)^4}\right) \\
&\tfrac{\hbar^2}{4m_D}(1+\alpha)^4 - 2Aa^2\alpha(1+\alpha) - A\alpha a^3(1+\alpha) + 3Aa^2\alpha^2 = 0 \\
&\tfrac{\hbar^2}{4m_D}(1+\alpha)^4 - 3Aa^2\alpha = 0 \\
&(1+\alpha)^4 - \beta\alpha = 0 \quad , \quad \beta = \tfrac{12m_D Aa^2}{\hbar^2}
\end{aligned}$$

Now

$$\begin{aligned}
&A = 32.7\,MeV = 32.7 \times 10^6 eV \cdot 1.602 \times 10^{-19} J/eV = 5.239 \times 10^{-12} J \\
&a^2 = (2.18 \times 10^{-13})cm^2 \cdot 10^{-4} m^2/cm^2 = 4.752 \times 10^{-30} m^2 \\
&\hbar^2 = (1.054 \times 10^{-34})^2 J^2 - s^2 = 1.111 \times 10^{-68} J^2 - s^2 \\
&m_D = \tfrac{m_n m_p}{m_n + m_p} = \tfrac{1.672 \cdot 1.670}{1.672 + 1.670} \times 10^{-27} kg = 0.835 \times 10^{-27} kg
\end{aligned}$$

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

$$\begin{aligned}
&\tfrac{\hbar^2}{4m_D a^2} = \tfrac{1.111}{4 \cdot 0.835 \cdot 4.752} \times 10^{-11} = 7.000 \times 10^{-13} J \\
&\to \tfrac{7.000 \times 10^{-13} J}{1.602 \times 10^{-13} J/MeV} = 4.369 MeV
\end{aligned}$$

and

$$\begin{aligned}
&E_0 \leq \tfrac{\alpha^2}{2}\left(4.369 - 65.4\tfrac{\alpha}{(1+\alpha)^3}\right) = 2.185\alpha^2 - 32.7\tfrac{\alpha^3}{(1+\alpha)^3} \\
&E_0 \leq 2.185(1.344)^2 - 32.7\left(\tfrac{1.344}{2.344}\right)^3 = 3.947 - 6.164 = -2.217 MeV
\end{aligned}$$

The experimentally measured value is $-2.23 MeV$.

9.5.6 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 $t > T$,

$$V = \frac{1}{2}m\omega^2 x^2$$

For $0 < t < T$,

$$V = \frac{1}{2}m\omega^2 (x-a)^2 = \frac{1}{2}m\omega^2 x^2 - m\omega^2 ax + \frac{1}{2}m\omega^2 a^2$$

For $t < 0$ and $t > T$,

$$H = H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \Rightarrow H_0 \left|\varphi_n\right\rangle = \hbar\omega(n+1/2)\left|\varphi_n\right\rangle$$

For $0 < t < T$,

$$\begin{aligned} H &= H_0 + W = \tfrac{p^2}{2m} + \tfrac{1}{2}m\omega^2 x^2 - m\omega^2 ax + \tfrac{1}{2}m\omega^2 a^2 \\ W &= -m\omega^2 ax + \tfrac{1}{2}m\omega^2 a^2 \end{aligned}$$

Therefore,

$$P_{fi} = \frac{1}{\hbar^2}\left|\int_0^T e^{i\omega_{fi}t'} W_{fi}(t')dt'\right|^2 \quad , \quad \omega_{fi} = \frac{1}{\hbar}(E_f - E_i)$$

Now,

$$\begin{aligned} W_{01} &= -m\omega^2 a \left\langle\varphi_0\right| x \left|\varphi_1\right\rangle + \frac{1}{2}m\omega^2 a^2 \left\langle\varphi_0 \mid \varphi_1\right\rangle \\ &= -m\omega^2 a\sqrt{\frac{\hbar}{2m\omega}}\left\langle\varphi_0\right|(a+a^+)\left|\varphi_1\right\rangle = -m\omega^2 a\sqrt{\frac{\hbar}{2m\omega}} \end{aligned}$$

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,

$$\begin{aligned} W_{21} &= -m\omega^2 a \left\langle\varphi_2\right| x \left|\varphi_1\right\rangle + \frac{1}{2}m\omega^2 a^2 \left\langle\varphi_2 \mid \varphi_1\right\rangle \\ &= -m\omega^2 a\sqrt{\frac{\hbar}{2m\omega}}\left\langle\varphi_2\right|(a+a^+)\left|\varphi_1\right\rangle = -m\omega^2 a\sqrt{\frac{\hbar}{m\omega}} \end{aligned}$$

so that

$$P_{21} = \frac{1}{\hbar^2}\left(-m\omega^2 a\sqrt{\frac{\hbar}{m\omega}}\right)^2 \left|\int_0^T e^{i\omega_{fi}t'}\,dt'\right|^2 = \frac{4m\omega a^2}{\hbar}\sin^2\left(\frac{\omega T}{2}\right)$$

In first-order perturbation theory, $P_{n1}\,(n > 2) = 0$ since $\langle\varphi_n|\,W\,|\varphi_1\rangle = 0$ for $n > 2$.

9.5.7 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

$$E_n = \hbar\bar{\omega}(n + 1/2) \quad , \quad \bar{\omega} = \sqrt{\frac{2k}{m}}$$

(b) What is the wave function in the ground state?

The ground-state wave function is

$$\langle x \mid \bar{0}\rangle = \psi_{\bar{o}}(x) = \left(\frac{m\bar{\omega}}{\pi\hbar}\right)^{1/4} e^{-\frac{m\bar{\omega}x^2}{2\hbar}}$$

(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

$$\langle x \mid 0\rangle = \psi_o(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} \quad , \quad \omega = \sqrt{\frac{k}{m}}$$

In this sudden approximation, we have

$$P(\text{remainsin}\,|\bar{0}\rangle) = \left|\langle \bar{0} \mid 0\rangle\right|^2 = \left|\int\limits_{-\infty}^{\infty} \psi_0(x)\psi_{\bar{0}}(x)dx\right|^2$$

$$= \left|\int\limits_{-\infty}^{\infty} \left(\frac{m\bar{\omega}}{\pi\hbar}\right)^{1/4} e^{-\frac{m\bar{\omega}x^2}{2\hbar}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} dx\right|^2$$

$$= \left(\frac{m\sqrt{\frac{2k}{m}}}{\pi\hbar}\right)^{1/2} \left(\frac{m\sqrt{\frac{k}{m}}}{\pi\hbar}\right)^{1/2} \left|\int\limits_{-\infty}^{\infty} e^{-\frac{m(\bar{\omega}+\omega)x^2}{2\hbar}} dx\right|^2$$

$$= 2^{1/4}\frac{m\sqrt{\frac{k}{m}}}{\pi\hbar} \frac{2\hbar}{m(\sqrt{2}+1)\sqrt{\frac{k}{m}}} \left|\int\limits_{-\infty}^{\infty} e^{-y^2} dy\right|^2$$

$$= \frac{2^{1/4}}{\pi} \frac{2}{(1+\sqrt{2})}\pi = 0.985$$

so the probability of remaining in the ground state is close to one.

9.5.8 Another perturbed oscillator

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

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

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

The initial state is $|0\rangle$. The transition amplitudes are

$$c_n^{(0)}(t) = \delta_{n0} \quad , \quad c_n^{(1)}(t) = -\frac{i}{\hbar}\int\limits_0^t e^{-i(E_0-E_n)t/\hbar} \langle n|\, H'(x,t)\, |0\rangle\, dt$$

Now,

$$\langle n|\, H'(x,t)\, |0\rangle = Ae^{-t/\tau} \langle n|\, x^2\, |0\rangle = Ae^{-t/\tau}\frac{\hbar}{2m\omega} \langle n|\, (a+a^+)(a+a^+)\, |0\rangle$$

$$= Ae^{-t/\tau}\frac{\hbar}{2m\omega} \langle n| \left(|0\rangle + \sqrt{2}\,|2\rangle\right) = Ae^{-t/\tau}\frac{\hbar}{2m\omega}\left(\delta_{n0} + \sqrt{2}\delta_{n2}\right)$$

Therefore, $c_n^{(1)}(t) = 0$ unless $n = 0, 2$. We therefore have that

$$c_0^{(0)}(t) = 0 = c_2^{(0)}(t)$$

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,

$$c_2^{(1)}(t) = -\frac{i}{\hbar} A \frac{\hbar}{2m\omega} \sqrt{2} \int_0^t e^{-i(E_0 - E_2)t/\hbar} e^{-t/\tau} dt = -\frac{iA\sqrt{2}}{2m\omega \left(\frac{1}{\tau} - 2\omega i \right)}$$

Thus, after a long time duration of the perturbation, the state becomes

$$|\psi\rangle = \left[1 - \frac{iA\tau}{2m\omega} \right] e^{-i\omega t/2} |0\rangle - \frac{iA\sqrt{2}}{2m\omega \left(\frac{1}{\tau} - 2\omega i \right)} e^{-i5\omega t/2} |2\rangle$$

(all higher order terms in A, that is, $A^2, A^3 < ......$ terms) are ignored).

Thus, the probability for the system to make a transition to the 2^{nd} excited state is

$$P_2 = \frac{|\langle 2 \mid \psi \rangle|^2}{\langle \psi \mid \psi \rangle} = \frac{\frac{A^2}{2m^2\omega^2\left(\frac{1}{\tau^2} + 4\omega^2\right)}}{\left[1 + \frac{iA^2\tau^2}{4m^2\omega^2} \right] + \frac{A^2}{2m\omega 2m^2\omega^2\left(\frac{1}{\tau^2} + 4\omega^2\right)}}$$

$$\approx \frac{A^2}{2m^2\omega^2 \left(\frac{1}{\tau^2} + 4\omega^2 \right)}$$

There is no probability for a transition to $|1\rangle$ or $|3\rangle$.

9.5.9 Nuclear Decay

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

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

where $\vec{r}$ is the electron coordinate.

(a) Write down the matrix element for the process in lowest-order perturbation theory, assuming that the electron is initially in a state characterized by the quantum numbers $(n\ell m)$, and that its energy, after it is emitted, is large enough so that its final state may be described by a plane wave, Neglect spin.

The initial state is

$$\varphi_0 = \psi_{n\ell m}(\vec{r})\varphi_i(\vec{r}_i, \vec{r}_2, ..., \vec{r}_Z)$$

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

$$W_{0\to 1} = \frac{2\pi}{\hbar} \rho(E_1) |W_{01}|^2 \delta(E_1 - E_0)$$

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 $n_x, n_y, n_z = 0, \pm 1, \pm 2, ...$ 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

$$dN = \frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3} = \frac{\text{volume of shell}}{\text{volume per state}}$$

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

$$W_{0\to 1} = \tfrac{2\pi}{\hbar}\tfrac{1}{4\pi^2}\left(\tfrac{2m}{\hbar^2}\right)^{3/2}\sqrt{E_1}$$
$$\times\left|\int d^3r e^{-i\vec{k}\cdot\vec{r}}\left\langle\varphi_f(\vec{r}_1,\vec{r}_2,...,\vec{r}_Z)\right|\sum_{j=1}^{Z}\tfrac{e^2}{|\vec{r}-\vec{r}_j|}\left|\varphi_i(\vec{r}_i,\vec{r}_2,...,\vec{r}_Z)\right\rangle\psi_{n\ell m}(\vec{r})\right|^2\delta(E_1-E_0)$$

(c) For light nuclei, the nuclear radius is much smaller than the Bohr radius for a give Z, and we can use the expansion

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

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

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

Using

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

we have

$$\langle\varphi_f(\vec{r}_1,\vec{r}_2,...,\vec{r}_Z)|\sum_{j=1}^{Z}\frac{e^2}{|\vec{r}-\vec{r}_j|}\,|\varphi_i(\vec{r}_i,\vec{r}_2,...,\vec{r}_Z)\rangle = \frac{e^2}{r^3}\vec{r}\cdot\langle\varphi_f(\vec{r}_1,\vec{r}_2,...,\vec{r}_Z)|\,\vec{r}_j\,|\varphi_i(\vec{r}_i,\vec{r}_2,...,\vec{r}_Z)\rangle = \frac{e^2}{r^3}\vec{r}\cdot\vec{d}$$

where $\vec{d}$ is independent of $\vec{r}$. We can therefore write

$$W_{0\to 1} = \frac{e^4}{2\pi\hbar}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E_1}\left|\vec{d}\cdot\int d^3r e^{-i\vec{k}\cdot\vec{r}}\frac{e^2}{r^3}\vec{r}\psi_{n\ell m}(\vec{r})\right|^2\delta(E_1-E_0)$$

Note that in the above result we have used

$$\frac{e^2}{r}\left\langle\varphi_f(\vec{r}_1,\vec{r}_2,...,\vec{r}_Z)\right|\hat{I}\left|\varphi_i(\vec{r}_i,\vec{r}_2,...,\vec{r}_Z)\right\rangle = 0$$

9.5.10 Time Evolution Operator

A one-dimensional anharmonic oscillator is given by the Hamiltonian

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

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

Using

$$O_I(t) = e^{iH_0t/\hbar} O e^{-iH_0t/\hbar}$$

and

$$[a, a^+] = 1$$

we get

$$\begin{aligned}
\frac{\partial a_I^+}{\partial t} &= \frac{i}{\hbar}[H_0, a_I^+] = \frac{i}{\hbar} e^{iH_0t/\hbar}[H_0, a^+]e^{-iH_0t/\hbar} \\
&= i\omega e^{iH_0t/\hbar}[a^+a, a^+]e^{-iH_0t/\hbar} = i\omega e^{iH_0t/\hbar}(a^+aa^+ - a^+a^+a)e^{-iH_0t/\hbar} \\
&= i\omega e^{iH_0t/\hbar}a^+[a, a^+]e^{-iH_0t/\hbar} = i\omega a_I^+
\end{aligned}$$

which implies that

$$a_I^+ = e^{i\omega t} a^+$$

which fulfills the condition $a_I^+(t = 0) = a^+$. We then have $a_I = e^{-i\omega t} a$

The perturbation in the interaction representation is then

$$V_I = \lambda a_I^+ a_I a_I = \lambda a^+ a a e^{-i\omega t}$$

The time evolution operator is now obtained to lowest order from

$$U(t, t_0) \approx I - \frac{i}{\hbar}\int_{t_0}^{t} dt' V_I = I - \frac{i\lambda}{\hbar} a^+ a a \int_{t_0}^{t} dt' e^{-i\omega t} = I - \frac{\lambda}{\hbar\omega} a^+ a a (e^{-i\omega t} - e^{-i\omega t_0})$$

9.5.11 Two-Level System

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

We have

$$\begin{aligned}
d_b &= \frac{i}{\hbar}\int_0^t \langle\psi_b| H'(t') |\psi_a\rangle e^{i\omega_{ba}t'} dt' \\
&= -\frac{i}{\hbar}\int_0^t \langle\psi_b| \hat{U}\delta(t') |\psi_a\rangle e^{i\omega_{ba}t'} dt' = -\frac{i}{\hbar} \langle\psi_b| \hat{U} |\psi_a\rangle
\end{aligned}$$

Then,

$$Prob_{(a\to b)} = |d_b|^2 = \frac{U^2}{\hbar^2}$$

9.5.12 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

$$H_{old} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \to \hbar\omega(a^+a + 1/2) \to |0\rangle_{old} = |0\rangle$$

and

$$H_{new} = \frac{(p+p_0)^2}{2m} + \frac{1}{2}m\omega^2 x^2 = H_{old} + \frac{p_0 p}{m} + \frac{p_0^2}{2m}$$

or

$$H_{new} = \hbar\omega(a^+a + 1/2) + \frac{p_0}{m}\sqrt{\frac{m\hbar\omega}{2}}(a - a^+) + \frac{p_0^2}{2m}$$

Now define $a = A + \beta$. This says that

$$[a, a^+] = 1 = [A, A^+]$$

and if we choose

$$\beta = i\frac{p_0}{m}\sqrt{\frac{m\hbar\omega}{2}}$$

$$H_{new} = \hbar\omega(A^+A + 1/2) + \frac{\hbar\omega}{4}$$

which is another harmonic oscillator with shifted energies.

The new ground state is defined by

$$A\,|0\rangle_{new} = 0 = (a - \beta)\,|0\rangle_{new}$$

or

$$a\,|0\rangle_{new} = \beta\,|0\rangle_{new}$$

Thus, $|0\rangle_{new}$ is a coherent state,i.e.,

$$|0\rangle_{new} = |\beta\rangle$$

where

$$a\,|\beta\rangle = \beta\,|\beta\rangle$$

Thus,

$$|0\rangle_{new} = e^{|\beta|^2/2}\sum_{m=0}^{\infty}\frac{\beta^m}{\sqrt{m!}}\,|m\rangle$$

Therefore,

$$\langle 0 \mid 0 \rangle_{new} = e^{|\beta|^2/2}$$

and the probability of remaining in the old ground state is

$$Prob = | \langle 0 \mid 0 \rangle_{new} |^2 = e^{|\beta|^2} = e^{-p_0^2/2m\hbar\omega}$$

9.5.13 Hydrogen beam between parallel plates

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

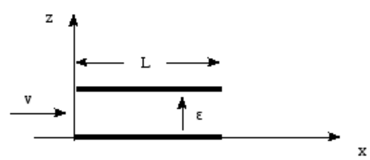


Figure 9.1: Hydrogen beam between parallel plates

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

(a) Which of the $n = 2$ states are connected (mixed) in first order via the electric field perturbation?

Consider the potential energy $e\mathcal{E}z$ of the electron (charge $= -e$) of a hydrogen atom in the external electric field $\mathcal{E}\hat{e}_z$ 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

$$\begin{pmatrix} 0 & \langle 200 | z | 210 \rangle & 0 & 0 \\ \langle 210 | z | 200 \rangle & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -3e\mathcal{E}a_0 & 0 & 0 \\ -3e\mathcal{E}a_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

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 2×2 submatrix are

$$E = 3e\mathcal{E}a_0 \to |+\rangle = \frac{1}{\sqrt{2}}(|200\rangle + |210\rangle) \quad , \quad E = -3e\mathcal{E}a_0 \to |-\rangle = \frac{1}{\sqrt{2}}(|200\rangle - |210\rangle)$$

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,

$$\begin{aligned}|\psi(t)\rangle &= \frac{1}{\sqrt{2}}\left(e^{i3e\mathcal{E}a_0 t/\hbar}|+\rangle + e^{-i3e\mathcal{E}a_0 t/\hbar}|-\rangle\right) = \begin{pmatrix}\cos(3e\mathcal{E}a_0 t/\hbar) \\ i\sin(3e\mathcal{E}a_0 t/\hbar)\end{pmatrix} \\ &= \cos(3e\mathcal{E}a_0 t/\hbar)|2s\rangle + i\sin(3e\mathcal{E}a_0 t/\hbar)|2p\rangle\end{aligned}$$

(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

$$\begin{aligned}|\langle 200 \mid \psi(t)\rangle|^2 &= |\langle 2s \mid \psi(t)\rangle|^2 = \cos^2(3e\mathcal{E}a_0 t/\hbar) \\ |\langle 210 \mid \psi(t)\rangle|^2 &= |\langle 2p \mid \psi(t)\rangle|^2 = \sin^2(3e\mathcal{E}a_0 t/\hbar)\end{aligned}$$

9.5.14 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:

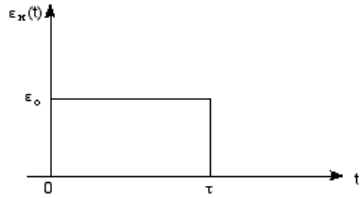


Figure 9.2: Electric Field

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

(a) Find the normalized bound-state energy eigenfunction corresponding to the delta function potential $V(x) = -A\delta(x)$.

The energy eigenfunction ψ satisfies the Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - A\delta(x)\psi = E\psi \quad , \quad E < 0$$

or

$$\frac{d^2\psi}{dx^2} - k^2\psi + A_0\delta(x)\psi = 0 \quad , \quad |E| = \frac{\hbar^2 k^2}{2m} \ , \ A_0 = \frac{2mA}{\hbar^2}$$

Integrating from $-\varepsilon \to +\varepsilon$, ε being an arbitrarily small, positive number and then letting $\varepsilon \to 0$, 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 Schrodinger equation has the solution

$$\psi(x) = Ce^{-k|x|}$$

so that

$$\psi(x) = Ce^{-kx} \ , \ x > 0 \quad , \quad \psi(x) = Ce^{kx} \ , \ x < 0$$

and thus

$$\frac{\psi'(0+)}{\psi(0+)} - \frac{\psi'(0-)}{\psi(0-)} = -2k \to k = \frac{A_0}{2} = \frac{mA}{\hbar^2}$$

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

$$e^{ikL/2} = e^{-ikL/2} \to e^{ikL} = 1 \to kL = 2n\pi \quad , \; n = 0, \pm 1, \pm 2, ...$$

so that

$$k_n = \frac{2n\pi}{L}$$

The normalized plane wave function for the wave vector k is

$$\psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx} = \frac{1}{\sqrt{L}} e^{i\frac{2n\pi}{L}x}$$

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,

$$E_k = \frac{\hbar^2 k^2}{2m} \to dE_k = \frac{\hbar^2 k}{m} dk \quad , \quad k = \frac{p}{\hbar} \to E_k = \frac{p^2}{2m}$$

or

$$\begin{array}{l} \frac{Ldp}{2\pi\hbar} = D(k)dk \to D(k) = \frac{L}{2\pi} \quad , \quad D(k)dk = \frac{1}{2} D(E_k) \frac{\hbar^2 k}{m} dk \\ D(E_k) = \frac{L}{\pi} \frac{m}{\hbar^2 k} = \frac{L}{\pi\hbar} \frac{m}{p} = \frac{L}{\pi\hbar} \frac{m}{\sqrt{2mE_k}} = \frac{L}{\pi\hbar} \sqrt{\frac{m}{2E_k}} \end{array}$$

(c) Assume that the electric field may be treated as a perturbation. Write down the perturbation term in the Hamiltonian, $\hat{H}_1$, and find the matrix element of $\hat{H}_1$ between the initial and the final state $\langle 0| \hat{H}_1 |k\rangle$.

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

$$\begin{aligned} \langle k| H' |0\rangle &= \int_{-\infty}^{\infty} \psi_k^* (-q\mathcal{E}_0 x) \psi dx = -\frac{q\mathcal{E}_0}{\sqrt{L}} \sqrt{\frac{mA}{\hbar^2}} \int_{-\infty}^{\infty} x e^{-ikx - k_0|x|} dx \\ &= -\frac{q\mathcal{E}_0}{\sqrt{L}} \sqrt{\frac{mA}{\hbar^2}} i \frac{d}{dk} \int_{-\infty}^{\infty} e^{-ikx-k_0|x|} dx = -\frac{q\mathcal{E}_0}{\sqrt{L}} \sqrt{\frac{mA}{\hbar^2}} i \frac{d}{dk} \left[\int_{-\infty}^{0} e^{-ikx+k_0x} dx + \int_{0}^{\infty} e^{-ikx-k_0x} dx \right] \\ &= -\frac{q\mathcal{E}_0}{\sqrt{L}} \sqrt{\frac{mA}{\hbar^2}} (-4ikk_0) \frac{1}{(k^2+k_0^2)^2} = \frac{4iq\mathcal{E}_0}{\sqrt{L}} \left(\frac{mA}{\hbar^2}\right)^{3/2} \frac{k}{\left(k^2 + \left(\frac{mA}{\hbar^2}\right)^2\right)^2} \end{aligned}$$

(d) The probability of a transition between an initially occupied state $|I\rangle$ and a final state $|F\rangle$ due to a weak perturbation $\hat{H}_1(t)$ is given by

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

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

The perturbation is

$$\hat{H}_1 = \begin{cases} 0 & -\infty < t < 0 \\ -q\mathcal{E}_0 x & 0 \le t \le \tau \\ 0 & t > \tau \end{cases}$$

The transition probability at $t > \tau$ is

$$\wp_{I\to F}(t) = \frac{1}{\hbar^2}\left|\langle k|\,\hat{H}_1\,|0\rangle\right|^2 \left|\int_0^{\tau} e^{i\omega_{FI}t'}dt'\right|^2 = \frac{1}{\hbar^2}\left|\langle k|\,\hat{H}_1\,|0\rangle\right|^2 \frac{\sin^2(\omega_{FI}\tau/2)}{(\omega_{FI}/2)^2}$$

Since

$$E_F = \frac{\hbar^2 k^2}{2m} \quad , \quad E_I = -\frac{mA^2}{2\hbar^2} \quad , \quad \omega_{FI} = \frac{1}{\hbar}(E_F - E_I)$$

we get

$$\frac{\sin^2(\omega_{FI}\tau/2)}{(\omega_{FI}/2)^2} = \frac{\sin^2\left(\frac{\hbar\tau}{4m}\left(k^2 + \left(\frac{mA}{\hbar^2}\right)^2\right)\right)}{\left(\frac{\hbar}{4m}\left(k^2 + \left(\frac{mA}{\hbar^2}\right)^2\right)\right)^2}$$

and the probability is given by

$$P(E_k)dE_k = \wp_{I\to F}(t)D(E_k)dE_k = \frac{1}{\hbar^2}\left|\langle k|\,\hat{H}_1\,|0\rangle\right|^2 \frac{\sin^2(\omega_{FI}\tau/2)}{(\omega_{FI}/2)^2}\frac{L}{\pi\hbar}\sqrt{\frac{m}{2E_k}}dE_k$$

$$= \frac{1}{\hbar^2}\left|\frac{4iq\mathcal{E}_0}{\sqrt{L}}\left(\frac{mA}{\hbar^2}\right)^{3/2}\frac{k}{\left(k^2 + \left(\frac{mA}{\hbar^2}\right)^2\right)^2}\right|^2 \frac{\sin^2(\omega_{FI}\tau/2)}{(\omega_{FI}/2)^2}\frac{L}{\pi\hbar}\sqrt{\frac{m}{2E_k}}dE_k$$

$$= \frac{1}{\hbar^2}\left|\frac{4iq\mathcal{E}_0}{\sqrt{L}}\left(\frac{mA}{\hbar^2}\right)^{3/2}\frac{k}{\left(k^2 + \left(\frac{mA}{\hbar^2}\right)^2\right)^2}\right|^2 \frac{\sin^2\left(\frac{\hbar\tau}{4m}\left(k^2 + \left(\frac{mA}{\hbar^2}\right)^2\right)\right)}{\left(\frac{\hbar}{4m}\left(k^2 + \left(\frac{mA}{\hbar^2}\right)^2\right)\right)^2}\frac{L}{\pi\hbar}\sqrt{\frac{m}{2E_k}}dE_k$$

9.5.15 Nasty time-dependent potential [complex integration needed]

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

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

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

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

$$\int F(t)dt$$

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

We have a perturbation potential

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

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

$$\omega_{10} = \frac{1}{\hbar}(E_1 - E_0) = \omega$$

We then have

$$c_1^{(1)}(\infty) = \frac{i}{h}\frac{F_0\tau}{\omega}\langle 1|\, x\,|0\rangle \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\tau^2 + t^2}dt$$

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

$$\lim_{R\to\infty} \oint \frac{e^{i\omega z}}{(z+i\tau)(z-i\tau)} = \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\tau^2+t^2}dt + \lim_{R\to\infty} \int_{semicircle} \frac{e^{i\omega z}}{(z+i\tau)(z-i\tau)} = 2\pi i \text{Residue}(z = i\tau)$$

$$\int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\tau^2+t^2}dt = 2\pi i \frac{e^{-\omega\tau}}{2i\tau} = \frac{\pi e^{-\omega\tau}}{\tau}$$

We also have

$$\langle 1| x |0\rangle = \sqrt{\frac{\hbar}{2m\omega}}$$

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

$$P_1 = \left|c_1^{(1)}(\infty)\right|^2 = \frac{\pi^2 F_0^2}{2mh\omega^3}e^{-2\omega\tau}$$

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 Schrodinger equation for the ground state.

9.5.16 Natural Lifetime of Hydrogen

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

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

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

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

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

The spontaneous decay rate on a dipole transition $|\psi_e\rangle \to |\psi_g\rangle$ summed over all possible final states is (Fermi Golden Rule)

$$\Gamma = \frac{4}{3\hbar}k^3\sum_g |\,\langle\psi_g|\,\hat{\vec{d}}|\psi_e\rangle\,|^2$$

Including the Hydrogen fine-structure

$$(nLJM_J) \to \sum_{M_J'}(n'L'J'M_J')$$

we have

$$\Gamma = \frac{4}{3\hbar}k^3 \sum_{M'_J} |\, \langle n'L'J'M'_J |\, \hat{\vec{d}} \,| nLJM_J \rangle \,|^2$$

(a) Show that the spontaneous emission rate is independent of the initial M_J. Explain this result physically.

Expand in the spherical basis

$$\hat{\vec{d}} = \sum_q \vec{e}_q^{\,*} \hat{d}_q$$

and use the Wigner-Eckhart theorem

$$\Gamma = \frac{4}{3\hbar}k^3 |\langle n'L'J' \| d \| nLJ \rangle|^2 \sum_{q,M_J} |\, \langle J'M'_J \,|\, 1qJM_j \rangle \,|^2$$

But

$$\sum_{q,M_J} |\, \langle J'M'_J \,|\, 1qJM_j \rangle \,|^2 = 1$$

by normalization. Therefore,

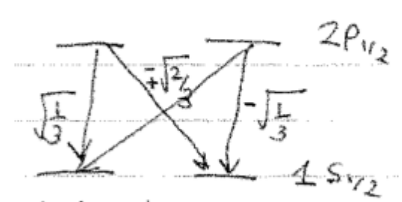
$$\Gamma = \frac{4}{3\hbar}k^3 |\langle n'L'J' \| d \| nLJ \rangle|^2$$

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 classical electromagnetic theory. The Larmor power (rate of energy from an oscillating dipole) goes as ω^3.

(b) Calculate the lifetime ($\tau = 1/\Gamma$) of the $2P_{1/2}$ state in seconds.

We have the allowed transitions with associated CG coefficients



where we note that the Lamb shift puts $2s_{1/2}$ above $2p_{1/2}$. 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 Γ 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.

$$\left\langle 1s_{1/2}, M_J = 1/2\right| \hat{d}_z \left|2p_{1/2}, M_J = 1/2\right\rangle = \rangle 1s_{1/2}\|d\|2p_{1/2}\rangle \left\langle 1/2, 1/2 \,|\, 101/21/2\right\rangle$$

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

$$\left|2p_{1/2}, 1/2\right\rangle = \sqrt{\tfrac{1}{3}}\left|2p, 0\right\rangle\left|1/2\right\rangle - \sqrt{\tfrac{2}{3}}\left|2p, 1\right\rangle\left|-1/2\right\rangle$$
$$\left|1s_{1/2}, 1/2\right\rangle = \left|1s, 0\right\rangle\left|1/2\right\rangle$$

This implies that

$$\left\langle 1s_{1/2}, M_J = 1/2\right| \hat{d}_z \left|2p_{1/2}, M_J = 1/2\right\rangle = \sqrt{\frac{1}{3}}\left\langle 1s, 0\right| \hat{d}_z \left|2p, 0\right\rangle = -\frac{e}{\sqrt{3}}\left\langle 1s, 0\right| \hat{z} \left|2p, 0\right\rangle$$

ASIDE: we have

$$\left\langle 1s, 0\right| \hat{z} \left|2p, 0\right\rangle = \int d^3x \psi^*_{2s,0}(\vec{x}) z \psi_{2p,0}(\vec{x})$$

and

$$z = \sqrt{\frac{4\pi}{3}} r Y_{10}(\theta, \phi)$$

Therefore,

$$\left\langle 1s, 0\right| \hat{z} \left|2p, 0\right\rangle = \sqrt{\frac{4\pi}{3}} \int_0^\infty dr\, u_{10} r u_{20} \int d\Omega Y_{00} Y_{10} Y_{10}$$

Now

$$\int_0^\infty dr\, u_{10} r u_{20} = \frac{a_0}{\sqrt{6}} \int_0^\infty dq q^4 e^{-3q/2} = 1.29 a_0$$

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,

$$\left\langle 1s_{1/2}, M_J = 1/2\right| \hat{d}_z \left|2p_{1/2}, M_J = 1/2\right\rangle = -\frac{e}{\sqrt{3}}\sqrt{\frac{4\pi}{3}}(1.29 a_0)\frac{1}{\sqrt{4\pi}} = -0.43 e a_0$$

Thus, we have

$$\rangle 1s_{1/2}\|d\|2p_{1/2}\rangle = \sqrt{3} 0.43 e a_0 = 0.74 e a_0$$

Thus,

$$\Gamma(2p_{1/2}) = (0.74)^2 \frac{4}{3\hbar} k^3 (ea_0)^2$$

In atomic units:

$$\begin{aligned}
&\tfrac{\hbar\Gamma}{e^2/a_0} = \tfrac{4}{3}(ka_0)^3 \left(\tfrac{\langle d \rangle}{ea_0}\right)^2 \\
&k = \tfrac{\omega}{c} = \tfrac{\hbar\omega}{\hbar c} = \epsilon \tfrac{E_0}{\hbar c} = \epsilon \tfrac{e^2}{\hbar c a_0} = \alpha\epsilon \tfrac{1}{a_0} \\
&\to \tfrac{\hbar\Gamma}{e^2/a_0} = \epsilon^3 \tfrac{4}{3}\alpha^3 \left(\tfrac{\langle d \rangle}{ea_0}\right)^2
\end{aligned}$$

Now,

$$\frac{\langle d \rangle}{ea_0} = 0.74 \quad , \quad \alpha = \frac{1}{137}$$

and for $n = 2 \to n = 1$,

$$\epsilon = \frac{\hbar\omega}{E_0} = \frac{3}{8}$$

Thus,

$$\frac{\hbar\Gamma}{e^2/a_0} = 1.5 \times 10^{-8}$$

Since

$$\frac{e^2}{a_0} = 27.2\, eV = 4.1 \times 10^{16}\, sec^{-1}$$

we get $\Gamma = 6.2 \times 10^8\, sec^{-1}$ and thus the lifetime is

$$\tau = \frac{1}{\Gamma} = 1.6\, ns$$

9.5.17 Oscillator in electric field

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

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

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

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

(a) What is the new ground state energy?

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 $a\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle$ where $\alpha = e\mathcal{E}x_o/\hbar\omega$, i.e.,

$$\left|0\right\rangle_{new} = \left|\alpha\right\rangle = e^{-|\alpha|^2/2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} \left|m\right\rangle$$

where

$$x_0 = \sqrt{\frac{\hbar}{2m\omega}}$$

The new ground state energy is the old ground state energy shifted by

$$-\frac{e^2\mathcal{E}^2 x_0^2}{\hbar\omega}$$

i.e.,

$$E_{0,new} = E_{0,old} - \frac{e^2\mathcal{E}^2 x_0^2}{\hbar\omega} = \frac{\hbar\omega}{2}\frac{e^2\mathcal{E}^2 x_0^2}{\hbar\omega}$$

(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

$$Prob = |\langle 0 \,|\, 0\rangle_{new}|^2 = e^{-|\alpha|^2}$$

9.5.18 Spin Dependent Transitions

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

$$\hat{V}_1 = \frac{1}{2}k\,|-\rangle\langle-| \otimes |\vec{r}|^2$$

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

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

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

(a) Suppose that a perturbation

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

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

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

We will denote states in the Hilbert space by

$$|\Psi\rangle = |s\rangle \otimes |\psi\rangle = |s;\psi\rangle$$

The first thing to do is to examine the potential

$$\hat{V}_1 = \frac{1}{2}k\,|-\rangle\,\langle-|\otimes|\vec{r}|^2$$

This potential corresponds to states of positive spin $|+\rangle$ being in a free potnetial and states of negative spin $|-\rangle$ being in a harmonic oscillator potential. The wave functions of the 3D harmonic oscillator can be obtain 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

$$E_{n_x n_y n_z} = \hbar\omega(n_x + n_y + n_z + 3/2) \quad n_x, n_y, n_z = 0, 1, 2, ...$$

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

$$a_{k+2} = 2\beta\frac{2k-4n}{(k+2)(k+2\ell+3)}a_k \quad k \geq 0,\ even$$

a_0 is determined by the normalization and $a_k = 0$ for all other k. The energies are

$$E_{n\ell m} = \hbar\omega(2n + \ell + 3/2) \quad n, \ell = 0, 1, 2, ... \quad m = -\ell, -\ell+1, ..., \ell-1, \ell$$

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

$$\langle\vec{x}\,|\,0\rangle = \psi_{n_x=0,n_y=0,n_z=0}(\vec{x}) = \psi_{n_x=0,\ell=0,m=0}(\vec{x}) = \left(\frac{m\omega}{2\hbar}\right)^{3/4} e^{-m\omega(x^2+y^2+z^2)/2\hbar} = \left(\frac{2\beta}{\pi}\right)^{3/4} e^{-\beta r^2}$$

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 $\left|\vec{k}\right\rangle$ and $|k\rangle$ to be the plane wave and spherical $s-$wave (respectively) with delta function normalizations:

$$\left\langle \vec{x} \,\middle|\, \vec{k} \right\rangle = \tfrac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}}$$
$$\left\langle \vec{k} \,\middle|\, \vec{k}' \right\rangle = \tfrac{1}{(2\pi)^3} \int d^3\vec{x} e^{i(\vec{k}\,'-\vec{k})\cdot\vec{x}} = \delta^3(\vec{k} - \vec{k}\,')$$
$$\langle \vec{x} \,|\, k \rangle = \tfrac{k}{\pi\sqrt{2}} j_0(kr) = \tfrac{1}{\pi\sqrt{2}} \tfrac{\sin(kr)}{r}$$
$$\langle k \,|\, k' \rangle = \tfrac{kk'}{2\pi^2} \int d^3\vec{x} [j_0(kr) j_0(k'r)] = \tfrac{2}{\pi} \int_0^\infty dr [\sin(kr) \sin(k'r)] = \delta(k - k')$$

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 $|\vec{k}| = k$ for the plane wave case):

$$\begin{aligned}
\left\langle 0 \,\middle|\, \vec{k} \right\rangle &= \int d^3\vec{x} \left(\frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}} \left(\frac{2\beta}{\pi}\right)^{3/4} e^{-\beta|\vec{x}|^2} \right) \\
&= \left(\frac{\beta}{2\pi^3}\right)^{3/4} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi \left(r^2 \sin\theta e^{ikr\cos\theta} e^{-\beta r^2} \right) \\
&= \left(\frac{\beta}{2\pi^3}\right)^{3/4} 2\pi \int_0^\infty dr \left(r^2 e^{-\beta r^2} \left. \frac{e^{ikr\cos\theta}}{-ikr} \right|_0^\pi \right) \\
&= \left(\frac{\beta}{2\pi^3}\right)^{3/4} \frac{4\pi}{k} \int_0^\infty \left(r \sin(kr) e^{-\beta r^2} \right) \\
&= \left(\frac{\beta}{2\pi^3}\right)^{3/4} \frac{4\pi}{k} I = \left(\frac{1}{2\pi\beta}\right)^{3/4} e^{-k^2/4\beta}
\end{aligned}$$

$$\begin{aligned}
\langle 0 \,|\, k \rangle &= \int d^3\vec{x} \left(\frac{k}{\pi\sqrt{2}} j_0(kr) \left(\frac{2\beta}{\pi}\right)^{3/4} e^{-\beta r^2} \right) \\
&= \left(\frac{2\beta}{\pi}\right)^{3/4} \frac{1}{\pi\sqrt{2}} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi \left(r^2 \sin\theta \frac{\sin(kr)}{r} e^{-\beta r^2} \right) \\
&= \left(\frac{2\beta}{\pi}\right)^{3/4} 2\sqrt{2} \int_0^\infty dr \left(r^2 \sin(kr) e^{-\beta r^2} \right) \\
&= \left(\frac{2\beta}{\pi}\right)^{3/4} 2\sqrt{2} I = \left(\frac{2}{\pi\beta}\right)^{3/4} \frac{k\sqrt{2\pi}}{2} e^{-k^2/4\beta}
\end{aligned}$$

where we have used the following evaluation of the integral:

$$\begin{aligned}
I &= \int_0^\infty dr \left(r^2 \sin(kr) e^{-\beta r^2} \right) \\
&= -\frac{1}{2\beta} \sin(kr) e^{-\beta r^2} \Big|_0^\infty + \frac{k}{2\beta} \int_0^\infty dr \left(\cos(kr) e^{-\beta r^2} \right) \\
&= \frac{k}{2\beta} \int_0^\infty dr \left(\cos(kr) e^{-\beta r^2} \right) = \frac{k}{2\beta} \int_0^\infty dr \left(\frac{e^{ikr} + e^{-ikr}}{2} e^{-\beta r^2} \right) \\
&= \frac{k}{4\beta} \left(\int_0^\infty dr e^{ikr} e^{-\beta r^2} + \int_{-\infty}^0 dr e^{ikr} e^{-\beta r^2} \right) \\
&= \frac{k}{4\beta} \int_{-\infty}^\infty dr e^{ikr} e^{-\beta r^2} = \frac{k}{4\beta} e^{-k^2/4\beta} \int_{-\infty}^\infty dr \left(e^{-\beta (r - ik/2\beta)^2} \right) \\
&= \frac{k\sqrt{\pi}}{4\beta^{3/2}} e^{-k^2/4\beta}
\end{aligned}$$

Now it remains to find the density of states for $\left|\vec{k}\right\rangle$ and $|k\rangle$.

For $\left|\vec{k}\right\rangle$, we use $\rho_f(\hat{k}, E) dE d\hat{k} = d^3\vec{k}$ where $\hat{k} = \vec{k}/|\vec{k}|$ 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:

$$\rho_f(\hat{k}, E) \frac{k^2 dk d\hat{k}}{dE d\hat{k}} = \frac{k^2 dk}{k^2 k dk/m} = \frac{mk}{\hbar^2} = \frac{\sqrt{2} m^{3/2}}{\hbar^3} E^{1/2}$$

Finally, we plug everything into Fermi's Golden Rule with

$$|\Psi_0\rangle = |-\rangle \otimes |0\rangle \quad , \quad |\Psi_{\vec{k}}\rangle = |+\rangle \otimes \left|\vec{k}\right\rangle$$

$$\vec{k}_0 = k_o \hat{k} \quad , \quad E_0 = \frac{\hbar^2 \_0^2}{2m} = \frac{3}{2} \hbar\omega$$

to get the transition rate:

$$\begin{aligned}
w(0 \to k_0) &= \frac{2\pi}{\hbar} |\langle \Psi_{k_0} | W | \Psi_0 \rangle|^2 \rho_f(E_0) = \frac{2\pi}{\hbar} (\hbar\Omega)^2 |\langle 0 \,|\, k_0 \rangle|^2 \rho_f(E_0) \\
&= 2\pi\hbar\Omega^2 \left(\frac{2}{\pi\beta} \right)^{3/2} e^{-k_0^2/2\beta} \frac{\sqrt{m}}{\hbar\sqrt{2}} E_0^{-1/2} \\
&= 2\pi\hbar\Omega^2 \left(\frac{4\hbar}{\pi m\omega} \right)^{3/2} \frac{3m\omega\pi}{2\hbar} e^{-3} \frac{\sqrt{m}}{\hbar\sqrt{2}} \left(\frac{3}{2} \hbar\omega \right)^{-1/2} \\
&= \frac{8\sqrt{3}}{e^3} \frac{\Omega^2}{\omega}
\end{aligned}$$

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 Ω.

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

$$\Sigma_+(\vec{x}) = \langle +;\vec{x}|\,\hat{V}_2\,|+;\vec{x}\rangle = \begin{cases} +\infty & |x| < a \\ 0 & |x| \geq a \end{cases}$$

$$\Sigma_-(\vec{x}) = \langle -;\vec{x}|\,\hat{V}_2\,|-;\vec{x}\rangle = \begin{cases} 0 & |x| < a \\ +\infty & |x| \geq a \end{cases}$$

(and spin off-diagonal terms of $\hat{V}_2$ being zero) requires that:

$\psi(\vec{x}) = \langle \vec{x}\,|\,\psi\rangle = 0$ in the region $|\vec{x}| \leq a$ for states with $s = +$

$\psi(\vec{x}) = \langle \vec{x}\,|\,\psi\rangle = 0$ in the region $|\vec{x}| \geq a$ 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 $\langle s_1|\,\hat{\sigma_x}\,|s_2\rangle = 1 - \delta_{s_1,s_2}$, this implies that

$$\begin{aligned}
\langle +;\psi|\,\hat{W}\,|+;\phi\rangle &= \hbar\Omega\,\langle +|\,\hat{\sigma_x}\,|+\rangle \textstyle\int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0 \\
\langle +;\psi|\,\hat{W}\,|-;\phi\rangle &= \hbar\Omega\,\langle +|\,\hat{\sigma_x}\,|-\rangle \textstyle\int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0 \\
\langle -;\psi|\,\hat{W}\,|+;\phi\rangle &= \hbar\Omega\,\langle -|\,\hat{\sigma_x}\,|+\rangle \textstyle\int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0 \\
\langle -;\psi|\,\hat{W}\,|-;\phi\rangle &= \hbar\Omega\,\langle -|\,\hat{\sigma_x}\,|-\rangle \textstyle\int \psi^*(\vec{x})\phi(\vec{x})d^3\vec{x} = 0
\end{aligned}$$

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 $\hat{V}_2$.

9.5.19 The Driven Harmonic Oscillator

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

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

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

(a) Using the lowest order perturbation theory to get a nonzero result, find the probability that the oscillator will be in the $2nd$ excited state $n = 2$ at time $t > 0$. Assume $\omega \neq \Omega$.

First-order:

$$d_f^{(1)} = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\langle f|\,H'(t')\,|i\rangle\,e^{i\omega_{fi}t'} = 0 \quad i = 0,\, f = 2$$

Second-order:

$$d_f^{(2)} = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \sum_n \langle f| H'(t') |n\rangle \langle n| H'(t'') |i\rangle e^{i\omega_{fn}t'} e^{i\omega_{ni}t''}$$

$$= \sum_n \frac{-F^2}{\hbar^2} \langle f| x |n\rangle \langle n| x |i\rangle \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' e^{i(\omega_{fn}-\Omega)t'} e^{i(\omega_{ni}-\Omega)t''}$$

For the harmonic oscillator,

$$\langle 2| x |n\rangle = x_0 \langle 2| (a + a^+) |n\rangle = x_0(\sqrt{n}\delta_{2,n-1} + \sqrt{n+1}\delta_{2,n+1})$$

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,

$$d_f^{(2)} = \frac{-F^2}{\hbar^2} \frac{\hbar}{2m\omega} \sqrt{2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' e^{i(\omega_{fn}-\Omega)t'} e^{i(\omega_{ni}-\Omega)t''}$$

Substituting $\omega_{20} = 2\omega$, $\omega_{10} = \omega$, $\omega_{21} = \omega$, we have (choosing $t_0 = 0$)

$$d_f^{(2)} = -\frac{F^2\sqrt{2}}{2m\omega\hbar} \frac{1}{(\omega-\Omega)^2} \frac{1}{2} \left(e^{2i(\omega-\Omega)t} - e^{i(\omega-\Omega)t} + 1\right)$$

Then, squaring, the probability is

$$P_{(0\to 2)} = |d_f|^2 = \frac{F^4}{2m^2\omega^2\hbar^2(\omega-\Omega)^4} \left(\frac{3}{2} + \frac{1}{2}\cos\left[2(\omega-\Omega)t\right] - 2\cos\left[(\omega-\Omega)t\right]\right)$$

(b) Now begin again and do the simpler case, $\omega = \Omega$. Again, find the probability that the oscillator will be in the $2nd$ excited state $n = 2$ at time $t > 0$

Using

$$d_f^{(2)} = \frac{-F^2\sqrt{2}}{2m\omega\hbar} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' e^{i(\omega_{fn}-\Omega)t'} e^{i(\omega_{ni}-\Omega)t''}$$

we now have the conditions $\omega_{21} = \Omega$, $\omega_{10} = \Omega$, so that (for $t_0 = 0$)

$$d_f^{(2)} = \frac{-F^2\sqrt{2}}{2m\omega\hbar} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' = \frac{-F^2\sqrt{2}}{2m\omega\hbar} \frac{t^2}{2}$$

Therefore, the probability is

$$P_{(0\to 2)} = \frac{F^4 t^4}{8\hbar^2 m^2 \omega^2}$$

(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

$$\begin{aligned} P_{(0\to 2)} &\approx \frac{F^4}{2m^2\omega^2\hbar^2(\omega-\Omega)^4}\left(\frac{3}{2}+\left(\frac{1}{2}-(\omega-\Omega)t^2+\frac{(\omega-\Omega)t^4}{3}\right)-\left(2-(\omega-\Omega)t^2+\frac{(\omega-\Omega)t^4}{12}\right)\right) \\ &= \frac{F^4t^4}{8\hbar^2m^2\omega^2} \end{aligned}$$

which is identical to the result obtained in part (b).

9.5.20 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 eigenvale 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

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

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

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) occuring 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)

$$\Gamma_{0\to 1} = \frac{2\pi}{\hbar}\frac{|\langle 1|\hat{V}|0\rangle|^2}{4}$$

See reasoning in Chapter 11.

(d) Given that $k = 3.0\,kg/s^2$, what photon wavelength is required to excite the electron from state ψ_0 to state ψ_1? Use symmetry arguments to decide whether this is an allowed transition (explain your reasoning); you might want to sketch $\psi_0(x)$ and $\psi_1(x)$ to help your explanation.

We have

$$\lambda = \frac{c}{\nu} = \frac{2\pi c}{\omega} = \frac{2\pi c\sqrt{m_e}}{\sqrt{k}}$$

(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,

$$\Gamma_{0\to 1} = \frac{2\pi}{\hbar}\frac{x_0^2}{4}$$

9.5.21 The Sudden Approximation

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

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

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

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

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

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

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

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

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 2α with the corresponding eigenstate

$$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Simple algebra on the remaining 2×2 submatrix gives the other eigenstates as

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

with eigenvalue 2α 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

$$f(t) = \frac{1}{2}\begin{pmatrix}1 & 0 & -1\end{pmatrix}\begin{pmatrix}e^{-i\alpha t} \\ 0 \\ -e^{-3i\alpha t}\end{pmatrix} = \frac{1}{2}(e^{-i\alpha t} + e^{-3i\alpha t})$$

and therefore

$$|f(t)|^2 = \frac{1}{2}(1 + \cos(2\alpha t))$$

which is indeed periodic with the largest Bohr frequency, which is $3\alpha - \alpha = 2\alpha$.

9.5.22 The Rabi Formula

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

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

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

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

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

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

Show that

$$|a(t)|^2 = \frac{(\gamma b_1)^2}{\Delta^2 + (\gamma b_1)^2}\sin^2\left(\frac{t}{2}\sqrt{\Delta^2 + (\gamma b_1)^2}\right)$$

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

In the rotating frame

$$|\psi'(0)\rangle = |\psi(t)\rangle = |-_z\rangle$$

and using results from the text (sections on magnetic resonance)

$$i\hbar\frac{d}{dt}\,|\psi'(t)\rangle = -\gamma\left(\left(B_0 + \frac{\omega}{\gamma}\right)S_z + b_1 S_x\right)|\psi'(t)\rangle$$

In matrix representation, we have

$$\frac{d}{dt}\begin{pmatrix}a \\ b\end{pmatrix} = -\frac{i}{2}\begin{pmatrix}\Delta & -\gamma b_1 \\ -\gamma b_1 & -\Delta\end{pmatrix}\begin{pmatrix}a \\ b\end{pmatrix}$$

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

$$\begin{pmatrix} -\frac{i\Delta}{2} - \lambda & \frac{i}{2}\gamma b_1 \\ \frac{i}{2}\gamma b_1 & \frac{i\Delta}{2} - \lambda \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

or

$$\left(-\frac{i\Delta}{2} - \lambda\right) a + \frac{i}{2}\gamma b_1 b = 0$$

or

$$a = -\frac{\gamma b_1}{i\Delta + 2\lambda} b$$

Thus, the unnormalized eigenstates and eigenvalues are

$$|a+\rangle = \begin{pmatrix} -i\gamma b_1 \\ i\Delta + i\sqrt{\Delta^2 + (\gamma b_1)^2} \end{pmatrix} \quad \leftrightarrow \quad +\frac{i}{2}\sqrt{\Delta^2 + (\gamma b_1)^2}$$

$$|a-\rangle = \begin{pmatrix} -i\gamma b_1 \\ i\Delta - i\sqrt{\Delta^2 + (\gamma b_1)^2} \end{pmatrix} \quad \leftrightarrow \quad -\frac{i}{2}\sqrt{\Delta^2 + (\gamma b_1)^2}$$

Thus,

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{2i\sqrt{\Delta^2 + (\gamma b_1)^2}}(|a+\rangle - |a-\rangle)$$

and so

$$\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \frac{1}{2i\sqrt{\Delta^2 + (\gamma b_1)^2}}(|a+\rangle\, e^{\frac{i}{2}\sqrt{\Delta^2+(\gamma b_1)^2}t} - |a-\rangle\, e^{-\frac{i}{2}\sqrt{\Delta^2+(\gamma b_1)^2}t})$$

and thus

$$\begin{aligned} a(t) &= -\frac{i\gamma b_1}{2i\sqrt{\Delta^2 + (\gamma b_1)^2}}(e^{\frac{i}{2}\sqrt{\Delta^2+(\gamma b_1)^2}t} - e^{-\frac{i}{2}\sqrt{\Delta^2+(\gamma b_1)^2}t}) \\ &= -\frac{i\gamma b_1}{2i\sqrt{\Delta^2 + (\gamma b_1)^2}}\left(2i\sin\left(\sqrt{\Delta^2 + (\gamma b_1)^2}\frac{t}{2}\right)\right) \\ &= -\frac{i\gamma b_1}{\sqrt{\Delta^2 + (\gamma b_1)^2}}\sin\left(\sqrt{\Delta^2 + (\gamma b_1)^2}\frac{t}{2}\right) \end{aligned}$$

and finally,

$$|a(t)|^2 = \frac{(\gamma b_1)^2}{\Delta^2 + (\gamma b_1)^2}\sin^2\left(\frac{t}{2}\sqrt{\Delta^2 + (\gamma b_1)^2}\right)$$

9.5.23 Rabi Frequencies in Cavity QED

Consider a two-level atom whose pure states can be represented by vectors in a two-dimensional Hilbert space $\mathcal{H}_A$. Let $|g\rangle$ and $|e\rangle$ be a pair of orthonormal basis states of $\mathcal{H}_A$ representing the ground and excited states of the atom, respectively. Consider also a microwave cavity whose lowest energy pure states can be described by vectors in a three-dimensional Hilbert space $\mathcal{H}_C$. Let $\{|0\rangle, |1\rangle, |2\rangle\}$

be orthonormal basis states representing zero, one and two microwave photons in the cavity.

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

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

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

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

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

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

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

$$\begin{aligned}
|E_0\rangle &= |g\rangle \otimes |0\rangle \\
|E_{1+}\rangle &= \frac{1}{\sqrt{2}}(|g\rangle \otimes |1\rangle + |e\rangle \otimes |0\rangle) \\
|E_{1-}\rangle &= \frac{1}{\sqrt{2}}(|g\rangle \otimes |1\rangle - |e\rangle \otimes |0\rangle) \\
|E_{2+}\rangle &= \frac{1}{\sqrt{2}}(|g\rangle \otimes |2\rangle + |e\rangle \otimes |1\rangle) \\
|E_{2-}\rangle &= \frac{1}{\sqrt{2}}(|g\rangle \otimes |2\rangle - |e\rangle \otimes |1\rangle)
\end{aligned}$$

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

$$H_{ac}|E_{1+}\rangle = \frac{\hbar\nu}{\sqrt{2}}(|e\rangle \otimes |0\rangle + |g\rangle \otimes |1\rangle) = \hbar\nu |E_{1+}\rangle \rightarrow E_{1+} = \hbar\nu$$

$$H_{ac}|E_{1-}\rangle = \frac{\hbar\nu}{\sqrt{2}}(|e\rangle \otimes |0\rangle - |g\rangle \otimes |1\rangle) = -\hbar\nu |E_{1+}\rangle \rightarrow E_{1-} = -\hbar\nu$$

$$H_{ac}|E_{2+}\rangle = \frac{\hbar\nu}{\sqrt{2}}(\sqrt{2}|e\rangle \otimes |1\rangle + \sqrt{2}|g\rangle \otimes |2\rangle) = \sqrt{2}\hbar\nu |E_{2+}\rangle \rightarrow E_{2+} = \sqrt{2}\hbar\nu$$

$$H_{ac}\,|E_{2-}\rangle = \frac{\hbar\nu}{\sqrt{2}}(\sqrt{2}\,|e\rangle\otimes|1\rangle - \sqrt{2}\,|g\rangle\otimes|2\rangle) = -\sqrt{2}\hbar\nu\,|E_{1+}\rangle \rightarrow E_{2-} = -\sqrt{2}\hbar\nu$$

By inspection we can write

$$\begin{aligned}|\psi(0)\rangle &= |g\rangle \otimes (c_0\,|0\rangle + c_1\,|1\rangle + c_2\,|2\rangle)\\ &= c_0\,|E_0\rangle + \frac{c_1}{\sqrt{2}}(|E_{1+}\rangle + |E_{1-}\rangle) + \frac{c_2}{\sqrt{2}}(|E_{2+}\rangle + |E_{2-}\rangle)\end{aligned}$$

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

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

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

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

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

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

$$\begin{aligned}P_e \otimes I^c\,|\psi(t)\rangle &= \frac{c_1}{2}(e^{-i\nu t} - e^{i\nu t})\,|e\rangle \otimes |0\rangle + \frac{c_2}{2}(e^{-\sqrt{2}i\nu t} - e^{\sqrt{2}i\nu t})\,|e\rangle \otimes |1\rangle\\ &= -ic_1\sin(\nu t)\,|e\rangle \otimes |0\rangle - ic_2\sin(\sqrt{2}\nu t)\,|e\rangle \otimes |1\rangle\end{aligned}$$

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.