

PHYS3701 Intro Quantum Mechanics I HW#1 Due 23 Jan 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) A beam of silver atoms is created by heating a vapor to 1500°C, and selecting atoms with a velocity close to the thermal mean value. The beam moves through a 1.5 m long magnetic field with a vertical gradient 8 T/m, and impinges a screen 2 m downstream of the end of the magnet. Assuming the silver atom has spin-1/2 with a magnetic moment of one Bohr magneton, find the separation distance in mm of the two states on the screen. *This is the calculation Stern and Gerlach had to do in order to design their experiment.*

(2) In class we wrote down the states $|\pm\hat{x}\rangle$ and $|\pm\hat{y}\rangle$ in terms of the two states $|\pm\hat{z}\rangle$. Using these expressions, show that

(a) $|\pm\hat{x}\rangle$ is orthogonal to $|\mp\hat{x}\rangle$

(b) $|\pm\hat{y}\rangle$ is orthogonal to $|\mp\hat{y}\rangle$

(c) The probability of measuring an electron to have its spin pointing in the $+\hat{y}$ direction, when the electron in fact is in the $|\mp\hat{z}\rangle$ state, is 1/2

(3) A spin-1/2 particle, say an electron, exists in the state

$$|\alpha\rangle = \frac{i}{2} |+\hat{z}\rangle - \frac{\sqrt{3}}{2} |-\hat{z}\rangle$$

What is the probability that a measurement of spin the $-\hat{y}$ direction gives the value $\hbar/2$?

(4) For an arbitrary unit vector $\hat{n} = \sin\theta \cos\phi \hat{x} + \sin\theta \sin\phi \hat{y} + \cos\theta \hat{z}$, I claim that

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

is the state for which a measurement of spin in the $+\hat{n}$ direction will always give $\hbar/2$. Construct the corresponding state $|-\hat{n}\rangle$ in terms of $|+\hat{z}\rangle$ and $|-\hat{z}\rangle$ by forcing it to be normalized, orthogonal to $|+\hat{n}\rangle$, and with a positive, real coefficient of $|+\hat{z}\rangle$. If you recognize that θ and ϕ are just the normal polar angles in three dimensions, can you see why you could have easily guessed your result for $|-\hat{n}\rangle$?

(5) Suppose you made a very large number of measurements of the spin in the \hat{z} direction for a bunch of electrons all in the state

$$|\alpha\rangle = \sqrt{\frac{1}{3}} |+\hat{z}\rangle + \sqrt{\frac{2}{3}} |-\hat{z}\rangle$$

In terms of \hbar , what would be the average value of all of your measurements?

(1) See the MATHEMATICA notebook. We find a separation of 6 mm.

(2) The expressions we came up with in class are

$$|\pm\hat{x}\rangle = \frac{1}{\sqrt{2}}|+\hat{z}\rangle \pm \frac{1}{\sqrt{2}}|-\hat{z}\rangle \quad \text{and} \quad |\pm\hat{y}\rangle = \frac{1}{\sqrt{2}}|+\hat{z}\rangle \pm \frac{i}{\sqrt{2}}|-\hat{z}\rangle$$

The dual vectors are given by

$$\langle\pm\hat{x}| = \frac{1}{\sqrt{2}}\langle+\hat{z}| \pm \frac{1}{\sqrt{2}}\langle-\hat{z}| \quad \text{and} \quad \langle\pm\hat{y}| = \frac{1}{\sqrt{2}}\langle+\hat{z}| \mp \frac{i}{\sqrt{2}}\langle-\hat{z}|$$

Now just form the inner products, so that

$$\begin{aligned} \langle-\hat{x}|+\hat{x}\rangle &= \left[\frac{1}{\sqrt{2}}\langle+\hat{z}| - \frac{1}{\sqrt{2}}\langle-\hat{z}| \right] \left[\frac{1}{\sqrt{2}}|+\hat{z}\rangle + \frac{1}{\sqrt{2}}|-\hat{z}\rangle \right] \\ &= \frac{1}{2}\langle+\hat{z}|+\hat{z}\rangle - \frac{1}{2}\langle-\hat{z}|+\hat{z}\rangle + \frac{1}{2}\langle+\hat{z}|-\hat{z}\rangle - \frac{1}{2}\langle-\hat{z}|-\hat{z}\rangle \\ &= \frac{1}{2}(1) - \frac{1}{2}(0) + \frac{1}{2}(0) - \frac{1}{2}(1) = 0 \\ \langle-\hat{y}|+\hat{y}\rangle &= \left[\frac{1}{\sqrt{2}}\langle+\hat{z}| + \frac{i}{\sqrt{2}}\langle-\hat{z}| \right] \left[\frac{1}{\sqrt{2}}|+\hat{z}\rangle + \frac{i}{\sqrt{2}}|-\hat{z}\rangle \right] \\ &= \frac{1}{2}\langle+\hat{z}|+\hat{z}\rangle + \frac{i}{2}\langle-\hat{z}|+\hat{z}\rangle + \frac{i}{2}\langle+\hat{z}|-\hat{z}\rangle - \frac{1}{2}\langle-\hat{z}|-\hat{z}\rangle \\ &= \frac{1}{2}(1) + \frac{i}{2}(0) + \frac{i}{2}(0) - \frac{1}{2}(1) = 0 \end{aligned}$$

The probability requested is given by

$$|\langle+\hat{y}|-\hat{z}\rangle|^2 = \left| \left[\frac{1}{\sqrt{2}}\langle+\hat{z}| + \frac{i}{\sqrt{2}}\langle-\hat{z}| \right] |-\hat{z}\rangle \right|^2 = \left| \frac{1}{\sqrt{2}}(0) + \frac{i}{\sqrt{2}}(1) \right|^2 = \frac{i}{\sqrt{2}} \frac{-i}{\sqrt{2}} = \frac{1}{2}$$

(3) The probability requested is given by

$$\begin{aligned} |\langle-\hat{y}|\alpha\rangle|^2 &= \left| \left[\frac{1}{\sqrt{2}}\langle+\hat{z}| + \frac{i}{\sqrt{2}}\langle-\hat{z}| \right] \left[\frac{i}{2}|+\hat{z}\rangle - \frac{\sqrt{3}}{2}|-\hat{z}\rangle \right] \right|^2 \\ &= \left| \frac{i}{2\sqrt{2}} - \frac{i\sqrt{3}}{2\sqrt{2}} \right|^2 = \frac{1}{8} (1 - \sqrt{3})^2 = \frac{2 - \sqrt{3}}{4} \approx 0.067 \end{aligned}$$

(4) Write $|- \hat{\mathbf{n}}\rangle = a|+\hat{\mathbf{z}}\rangle + b|-\hat{\mathbf{z}}\rangle$ where $|a|^2 + |b|^2 = 1$ and a is real and positive. Imposing the orthogonality condition means $\langle +\hat{\mathbf{n}}| - \hat{\mathbf{n}}\rangle = 0$, so

$$a \cos \frac{\theta}{2} + b e^{-i\phi} \sin \frac{\theta}{2} = 0 \quad \text{therefore} \quad b = -a e^{i\phi} \cot \frac{\theta}{2}$$

We can then calculate

$$a^2 + a^2 \cot^2 \frac{\theta}{2} = a^2 \left[1 + \frac{\cos^2 \theta/2}{\sin^2 \theta/2} \right] = \frac{a^2}{\sin^2 \theta/2} = 1 \quad \text{so} \quad a = \sin \frac{\theta}{2}$$

where we note that $0 \leq \theta \leq \pi$ so that $a > 0$ for all θ . Therefore, we find that

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

which agrees with Problem 1.6 in Townsend.

It is clear that in order to flip $+\hat{\mathbf{n}}$ to the opposite direction, we take $\theta \rightarrow \pi - \theta$ and $\phi \rightarrow \phi + \pi$, so we would have naturally expected that

$$|- \hat{\mathbf{n}}\rangle = \cos \frac{\pi - \theta}{2} |+\hat{\mathbf{z}}\rangle + e^{i(\phi + \pi)} \sin \frac{\pi - \theta}{2} |-\hat{\mathbf{z}}\rangle = \sin \frac{\theta}{2} |+\hat{\mathbf{z}}\rangle - e^{i\phi} \cos \frac{\theta}{2} |-\hat{\mathbf{z}}\rangle$$

(5) The probability of measuring $+\hbar/2$ is $1/3$, and the probability of measuring $-\hbar/2$ is $2/3$, so after a large number of measurements, the average value will be

$$\frac{1}{3} \left(+\frac{\hbar}{2} \right) + \frac{2}{3} \left(-\frac{\hbar}{2} \right) = \frac{\hbar}{6} (1 - 2) = -\frac{\hbar}{6}$$

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PHYS3701 Intro Quantum Mechanics I HW#2 Due 30 Jan 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) The *trace* of an operator X is defined as

$$\text{Tr}(X) = \sum_{a'} \langle a' | X | a' \rangle$$

where the $|a'\rangle$ are a set of eigenstates based on some Hermitian operator A . Prove that

- (a) $\text{Tr}(X) = \sum_{b'} \langle b' | X | b' \rangle$ where the $|b'\rangle$ are any other complete set of eigenvectors, that is, it doesn't matter which basis you use to evaluate the trace.
- (b) $\text{Tr}(XY) = \text{Tr}(YX)$ for any two operators X and Y .

You will find it useful to invoke completeness by “inserting the identity operator.”

(2) Using the outer product expressions for the spin operators derived in class, show that

$$S_x S_y = -S_y S_x \quad \text{and} \quad [S_x, S_y] \equiv S_x S_y - S_y S_x = i\hbar S_z$$

(3) In a certain two state system, an operator H has the form

$$H = a|1\rangle\langle 1| + a|2\rangle\langle 2| + ib|1\rangle\langle 2| - ib|2\rangle\langle 1|$$

where a and b are real numbers.

- (a) Show that H is Hermitian.
 - (b) Find the eigenvalues of H in terms of a and b and show that they are real.
 - (c) Find the eigenvectors of H in terms of a , b , $|1\rangle$, and $|2\rangle$. Normalize the eigenvectors, but you should find that this is simple.
- (4) For an arbitrary unit vector $\hat{\mathbf{n}} = \sin\theta \cos\phi \hat{\mathbf{x}} + \sin\theta \sin\phi \hat{\mathbf{y}} + \cos\theta \hat{\mathbf{z}}$, form the spin-1/2 operator $S_n = \vec{\mathbf{S}} \cdot \hat{\mathbf{n}}$. Show that the eigenvalues of S_n are exactly what you expect. Find the eigenvectors and compare to your answer for Problem 4 on Homework 1.
- (5) Calculate expectation value of the operator S_z , that is $\langle S_z \rangle$, for the spin-1/2 state

$$|\alpha\rangle = \sqrt{\frac{1}{3}} |+\hat{\mathbf{z}}\rangle + \sqrt{\frac{2}{3}} |-\hat{\mathbf{z}}\rangle$$

and compare to your answer for Problem 5 on Homework 1. Then calculate the expectation values $\langle S_x \rangle$ and $\langle S_y \rangle$.

(1) Making use of the operator $1 = \sum_{b'} |b'\rangle\langle b'| = \sum_{b''} |b''\rangle\langle b''|$ we write

$$\begin{aligned} \text{Tr}(X) &= \sum_{a'} \langle a'|X|a'\rangle = \sum_{a'} \langle a'|1X1|a'\rangle = \sum_{a'} \sum_{b'} \sum_{b''} \langle a'|b'\rangle \langle b'|X|b''\rangle \langle b''|a'\rangle \\ &= \sum_{a'} \sum_{b'} \sum_{b''} \langle b''|a'\rangle \langle a'|b'\rangle \langle b'|X|b''\rangle = \sum_{b'} \sum_{b''} \langle b''|1|b'\rangle \langle b'|X|b''\rangle \\ &= \sum_{b'} \sum_{b''} \langle b''|b'\rangle \langle b'|X|b''\rangle = \sum_{b'} \sum_{b''} \delta_{b'',b'} \langle b'|X|b''\rangle = \sum_{b'} \langle b'|X|b'\rangle \end{aligned}$$

$$\begin{aligned} \text{and } \text{Tr}(XY) &= \sum_{a'} \langle a'|XY|a'\rangle = \sum_{a'} \langle a'|X1Y|a'\rangle \\ &= \sum_{a'} \sum_{b'} \langle a'|X|b'\rangle \langle b'|Y|a'\rangle = \sum_{a'} \sum_{b'} \langle b'|Y|a'\rangle \langle a'|X|b'\rangle \\ &= \sum_{b'} \langle b'|Y1X|b'\rangle = \sum_{b'} \langle b'|YX|b'\rangle = \text{Tr}(YX) \end{aligned}$$

(2) Just do the work and the answers fall out. First the commutator, so

$$\begin{aligned} S_x S_y &= \left(\frac{\hbar}{2} [|\hat{z}\rangle\langle -\hat{z}| + |-\hat{z}\rangle\langle \hat{z}|] \right) \left(\frac{\hbar}{2} [-i|\hat{z}\rangle\langle -\hat{z}| + i|-\hat{z}\rangle\langle \hat{z}|] \right) \\ &= \frac{\hbar^2}{4} (0 + i|\hat{z}\rangle\langle \hat{z}| - i|-\hat{z}\rangle\langle -\hat{z}| + 0) \\ &= \frac{\hbar^2}{4} [i|\hat{z}\rangle\langle \hat{z}| - i|-\hat{z}\rangle\langle -\hat{z}|] \\ S_y S_x &= \left(\frac{\hbar}{2} [-i|\hat{z}\rangle\langle -\hat{z}| + i|-\hat{z}\rangle\langle \hat{z}|] \right) \left(\frac{\hbar}{2} [|\hat{z}\rangle\langle -\hat{z}| + |-\hat{z}\rangle\langle \hat{z}|] \right) \\ &= \frac{\hbar^2}{4} (0 - i|\hat{z}\rangle\langle \hat{z}| + i|-\hat{z}\rangle\langle -\hat{z}| + 0) \\ &= \frac{\hbar^2}{4} [-i|\hat{z}\rangle\langle \hat{z}| + i|-\hat{z}\rangle\langle -\hat{z}|] = -S_x S_y \end{aligned}$$

$$\begin{aligned} \text{and } [S_x, S_y] &= S_x S_y - S_y S_x \\ &= 2i \frac{\hbar^2}{4} [|\hat{z}\rangle\langle \hat{z}| - |-\hat{z}\rangle\langle -\hat{z}|] = i\hbar S_z \end{aligned}$$

(3) It is obvious that H is Hermitian, since taking the adjoint flips the bras and kets and takes the complex conjugates of the coefficients. The eigenvalue problem reduces to solving for λ using

$$\begin{vmatrix} a - \lambda & ib \\ -ib & a - \lambda \end{vmatrix} = (a - \lambda)^2 - b^2 = 0 \quad \text{so} \quad \lambda = a \pm b$$

which are clearly real numbers. For $\lambda = a + b$, we have

$$\begin{bmatrix} -b & ib \\ -ib & -b \end{bmatrix} \begin{bmatrix} u_1^{(+)} \\ u_2^{(+)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \text{so} \quad -u_1^{(+)} + iu_2^{(+)} = 0 \quad \text{or} \quad -iu_1^{(+)} - u_2^{(+)} = 0$$

which both say that $u_2^{(+)} = -iu_1^{(+)}$. For $\lambda = a - b$, we have

$$\begin{bmatrix} b & ib \\ -ib & b \end{bmatrix} \begin{bmatrix} u_1^{(-)} \\ u_2^{(-)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \text{so} \quad u_1^{(-)} + iu_2^{(-)} = 0 \quad \text{or} \quad -iu_1^{(-)} + u_2^{(-)} = 0$$

which both say that $u_2^{(-)} = -iu_1^{(-)}$. The normalized eigenkets are therefore

$$|a + b\rangle = \frac{1}{\sqrt{2}} [|1\rangle - i|2\rangle] \quad \text{and} \quad |a - b\rangle = \frac{1}{\sqrt{2}} [|1\rangle + i|2\rangle]$$

(4) Using the matrix representation in the $|\pm\hat{z}\rangle$ basis, we have

$$\begin{aligned} S_n &= \sin\theta \cos\phi \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \sin\theta \sin\phi \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + \cos\theta \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ &= \frac{\hbar}{2} \begin{bmatrix} \cos\theta & \sin\theta \cos\phi - i \sin\theta \sin\phi \\ \sin\theta \cos\phi + i \sin\theta \sin\phi & -\cos\theta \end{bmatrix} \\ &= \frac{\hbar}{2} \begin{bmatrix} \cos\theta & e^{-i\phi} \sin\theta \\ e^{i\phi} \sin\theta & -\cos\theta \end{bmatrix} \end{aligned}$$

The eigenvalues are therefore $(\hbar/2)\lambda$ where we get λ by solving

$$\begin{vmatrix} \cos\theta - \lambda & e^{-i\phi} \sin\theta \\ e^{i\phi} \sin\theta & -\cos\theta - \lambda \end{vmatrix} = -(\cos^2\theta - \lambda^2) - \sin^2\theta = -1 + \lambda^2 = 0$$

so $\lambda = \pm 1$ and the eigenvalues are $\pm\hbar/2$, as expected. To get the eigenvectors, it is convenient to write

$$\cos\theta - 1 = -2\sin^2\frac{\theta}{2} \quad \cos\theta + 1 = 2\cos^2\frac{\theta}{2} \quad \text{and} \quad \sin\theta = 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$$

In this case, the eigenvector coefficients for $\lambda = +1$ come from solving

$$\begin{bmatrix} -2\sin^2(\theta/2) & e^{-i\phi}2\sin(\theta/2)\cos(\theta/2) \\ e^{i\phi}2\sin(\theta/2)\cos(\theta/2) & 2\cos^2(\theta/2) \end{bmatrix} \begin{bmatrix} u_1^{(+)} \\ u_2^{(+)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

both of which give $u_2^{(+)} = u_1^{(+)} e^{i\phi} \sin(\theta/2) / \cos(\theta/2)$. Normalization gives

$$\left(u_1^{(+)}\right)^2 \left[1 + \frac{\sin^2(\theta/2)}{\cos^2(\theta/2)}\right] = \left(u_1^{(+)}\right)^2 \frac{1}{\cos^2(\theta/2)} = 1$$

so we have $u_1^{(+)} = \cos(\theta/2)$ and $u_2^{(+)} = e^{i\phi} \sin(\theta/2)$, which agrees with the statement in Problem 4 in Homework 1. For $\lambda = -1$ we get

$$\begin{bmatrix} 2\cos^2(\theta/2) & e^{-i\phi}2\sin(\theta/2)\cos(\theta/2) \\ e^{i\phi}2\sin(\theta/2)\cos(\theta/2) & 2\sin^2(\theta/2) \end{bmatrix} \begin{bmatrix} u_1^{(+)} \\ u_2^{(+)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

both of which give $u_2^{(+)} = -u_1^{(+)} e^{i\phi} \cos(\theta/2) / \sin(\theta/2)$. Normalization gives

$$\left(u_1^{(+)}\right)^2 \left[1 + \frac{\cos^2(\theta/2)}{\sin^2(\theta/2)}\right] = \left(u_1^{(+)}\right)^2 \frac{1}{\sin^2(\theta/2)} = 1$$

so we have $u_1^{(+)} = \sin(\theta/2)$ and $u_2^{(+)} = -e^{i\phi} \cos(\theta/2)$, which agrees with the solution to Problem 4 in Homework 1.

(5) Calculating the expectation value $\langle S_z \rangle$ just parallels what we did in Homework 1, namely

$$\begin{aligned}
 \langle S_z \rangle &= \langle \alpha | S_z | \alpha \rangle \\
 &= \left[\sqrt{\frac{1}{3}} \langle +\hat{z} | + \sqrt{\frac{2}{3}} \langle -\hat{z} | \right] \frac{\hbar}{2} (|+\hat{z}\rangle \langle +\hat{z}| - |-\hat{z}\rangle \langle -\hat{z}|) \left[\sqrt{\frac{1}{3}} |+\hat{z}\rangle + \sqrt{\frac{2}{3}} |-\hat{z}\rangle \right] \\
 &= \frac{\hbar}{2} \left[\sqrt{\frac{1}{3}} \langle +\hat{z} | - \sqrt{\frac{2}{3}} \langle -\hat{z} | \right] \left[\sqrt{\frac{1}{3}} |+\hat{z}\rangle + \sqrt{\frac{2}{3}} |-\hat{z}\rangle \right] \\
 &= \frac{\hbar}{2} \left(\frac{1}{3} \right) - \frac{\hbar}{2} \left(\frac{2}{3} \right) = -\frac{\hbar}{6}
 \end{aligned}$$

The calculations for $\langle S_x \rangle$ and $\langle S_y \rangle$ are similarly easy.

$$\begin{aligned}
 \langle S_x \rangle &= \langle \alpha | S_x | \alpha \rangle \\
 &= \left[\sqrt{\frac{1}{3}} \langle +\hat{z} | + \sqrt{\frac{2}{3}} \langle -\hat{z} | \right] \frac{\hbar}{2} (|+\hat{z}\rangle \langle -\hat{z}| + |-\hat{z}\rangle \langle +\hat{z}|) \left[\sqrt{\frac{1}{3}} |+\hat{z}\rangle + \sqrt{\frac{2}{3}} |-\hat{z}\rangle \right] \\
 &= \frac{\hbar}{2} \left[\sqrt{\frac{1}{3}} \langle -\hat{z} | + \sqrt{\frac{2}{3}} \langle +\hat{z} | \right] \left[\sqrt{\frac{1}{3}} |+\hat{z}\rangle + \sqrt{\frac{2}{3}} |-\hat{z}\rangle \right] \\
 &= \frac{\hbar}{2} \frac{\sqrt{2}}{3} + \frac{\hbar}{2} \frac{\sqrt{2}}{3} = \hbar \frac{\sqrt{2}}{3} \\
 \langle S_y \rangle &= \langle \alpha | S_y | \alpha \rangle \\
 &= \left[\sqrt{\frac{1}{3}} \langle +\hat{z} | + \sqrt{\frac{2}{3}} \langle -\hat{z} | \right] \frac{\hbar}{2} (-i |+\hat{z}\rangle \langle -\hat{z}| + i |-\hat{z}\rangle \langle +\hat{z}|) \left[\sqrt{\frac{1}{3}} |+\hat{z}\rangle + \sqrt{\frac{2}{3}} |-\hat{z}\rangle \right] \\
 &= \frac{\hbar}{2} \left[-i \sqrt{\frac{1}{3}} \langle -\hat{z} | + i \sqrt{\frac{2}{3}} \langle +\hat{z} | \right] \left[\sqrt{\frac{1}{3}} |+\hat{z}\rangle + \sqrt{\frac{2}{3}} |-\hat{z}\rangle \right] \\
 &= -i \frac{\hbar}{2} \sqrt{\frac{2}{3}} + i \frac{\hbar}{2} \sqrt{\frac{2}{3}} = 0
 \end{aligned}$$

PHYS3701 Intro Quantum Mechanics I HW#3 Due 6 Feb 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) Consider the possibility of an observable P for which the Hermitian operator is also unitary, that is $P^\dagger = P = P^{-1}$. Show that this implies that $P^2 = 1$. Can you think of a practical real world example of such an operator in three-dimensional space?

(2) For a certain two-state system, the Hamiltonian has the time-independent form

$$H = |1\rangle\delta\langle 2| + |2\rangle\delta\langle 1|$$

where δ is a real number. Calculate the eigenvalues and eigenstates of H , and find the time-evolved state $|\alpha; t\rangle$ assuming the system starts out in the state $|\alpha\rangle = |1\rangle$. Determine the probability that a measurement finds the system in $|1\rangle$ as a function of time.

(3) A spin-1/2 particle with charge q sits in a static magnetic field $\vec{\mathbf{B}} = B\hat{z}$. The particle is initially in the state $|+\hat{x}\rangle$, that is, the state for which a measurement of the spin in the $+\hat{x}$ direction will always give $+\hbar/2$. Find the expectation value $\langle S_y \rangle$ as a function of time and argue that your answer is exactly what you expect.

(4) An electron is subject to a static magnetic field $\vec{\mathbf{B}} = B\hat{z}$. At $t = 0$ the electron is known to be in an eigenstate of $S_n = \vec{\mathbf{S}} \cdot \hat{\mathbf{n}}$ with eigenvalue $+\hbar/2$, where $\hat{\mathbf{n}}$ is a unit vector, lying in the xz -plane, that makes an angle θ with the z -axis.

- (a) Find the probability for finding the electron in the $|+\hat{x}\rangle$ state as a function of time.
- (b) Find the expectation value of S_x as a function of time.
- (c) Show that your answers make good sense for $\theta = 0$ and $\theta = \pi/2$.

You can make use of your results on Problem 4 of Homework 2.

(5) Neutrinos are very low mass particles that are only detected through the so-called weak interaction, and are observed only in the eigenstates

$$|\nu_e\rangle = \cos\theta|\nu_1\rangle - \sin\theta|\nu_2\rangle \quad \text{and} \quad |\nu_\mu\rangle = \sin\theta|\nu_1\rangle + \cos\theta|\nu_2\rangle$$

where $|\nu_1\rangle$ and $|\nu_2\rangle$ are eigenstates of the (full) Hamiltonian with masses m_1 and m_2 and θ is a “mixing angle.” Making the assumption that electron neutrinos are produced with definite momentum $p \gg mc$ and energy $E = (p^2c^2 + m^2c^4)^{1/2}$ at time $t = 0$, show that the probability of detecting the neutrino as an electron neutrino at some distance L is given by

$$P(\nu_e \rightarrow \nu_e) = 1 - \sin^2 2\theta \sin^2 \left(\Delta m^2 c^4 \frac{L}{4E\hbar c} \right)$$

where $\Delta m^2 \equiv m_1^2 - m_2^2$. Now look up the paper “Precision Measurement of Reactor Antineutrino Oscillation at Kilometer-Scale Baselines by Daya Bay”, by F.P. An, *et al.*, Phys. Rev. Lett. 130, 161802, and use Figure 3 to estimate the sizes of $\Delta m^2 c^2$ (in eV²) and $\sin^2 2\theta$, which you can compare the the results published in the paper.

(1) It is simple to show that $P^2 = PP = P^{-1}P = 1$. In other words, do the operation twice and you come back to where you started. The classic (and important) example is the parity operation, where the position vector $\vec{r} \rightarrow -\vec{r}$.

(2) Find the eigenvalues and eigenvectors by diagonalizing H in the given basis. That is

$$\begin{bmatrix} 0 & \delta \\ \delta & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = E \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \quad \text{so} \quad \begin{vmatrix} -E & \delta \\ \delta & -E \end{vmatrix} = E^2 - \delta^2 = 0$$

and the eigenvalues are just $E_1 = +\delta$, for which $v_2 = v_1$, and $E_2 = -\delta$, for which $v_2 = -v_1$. Therefore the eigenstates are

$$|E_1\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle \quad \text{and} \quad |E_2\rangle = \frac{1}{\sqrt{2}}|1\rangle - \frac{1}{\sqrt{2}}|2\rangle \quad \text{so} \quad |1\rangle = \frac{1}{\sqrt{2}}|E_1\rangle + \frac{1}{\sqrt{2}}|E_2\rangle$$

We can now apply the time evolution operator to get

$$|\alpha; t\rangle = U(t)|\alpha; t=0\rangle = e^{-iHt/\hbar}|1\rangle = e^{-iHt/\hbar} \left[\frac{1}{\sqrt{2}}|E_1\rangle + \frac{1}{\sqrt{2}}|E_2\rangle \right] = \frac{e^{-iE_1t/\hbar}}{\sqrt{2}}|E_1\rangle + \frac{e^{-iE_2t/\hbar}}{\sqrt{2}}|E_2\rangle$$

and the probability of finding the particle in the state $|1\rangle$ is

$$P = |\langle 1|\alpha; t\rangle|^2 = \left| \frac{e^{-iE_1t/\hbar}}{\sqrt{2}}\langle 1|E_1\rangle + \frac{e^{-iE_2t/\hbar}}{\sqrt{2}}\langle 1|E_2\rangle \right|^2 = \frac{1}{4} |e^{-i\delta t/\hbar} + e^{+i\delta t/\hbar}|^2 = \cos^2 \left(\frac{\delta t}{\hbar} \right)$$

(3) This is very similar to what we worked through in class. The Hamiltonian is

$$H = -\frac{q}{mc} \vec{S} \cdot \vec{B} = -\omega S_z \quad \text{with} \quad \omega \equiv \frac{qB}{mc}$$

The time translation operator is therefore

$$U(t) = \exp \left(-\frac{iHt}{\hbar} \right) = \exp \left(\frac{i\omega S_z t}{\hbar} \right)$$

The state of the particle at time t is just given by

$$|\alpha; t\rangle = U(t)|+\hat{x}\rangle = \exp \left(\frac{i\omega S_z t}{\hbar} \right) \left[\frac{1}{\sqrt{2}}|+\hat{z}\rangle + \frac{1}{\sqrt{2}}|-\hat{z}\rangle \right] = \frac{e^{i\omega t/2}}{\sqrt{2}}|+\hat{z}\rangle + \frac{e^{-i\omega t/2}}{\sqrt{2}}|-\hat{z}\rangle$$

It's probably easiest to calculate the expectation value using the matrix representation, so

$$\begin{aligned} \langle S_y \rangle &= \langle \alpha; t | S_y | \alpha; t \rangle = \begin{bmatrix} e^{-i\omega t/2}/\sqrt{2} & e^{i\omega t/2}/\sqrt{2} \end{bmatrix} \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} e^{i\omega t/2}/\sqrt{2} \\ e^{-i\omega t/2}/\sqrt{2} \end{bmatrix} \\ &= \frac{\hbar}{2} \begin{bmatrix} ie^{i\omega t/2}/\sqrt{2} & -ie^{-i\omega t/2}/\sqrt{2} \end{bmatrix} \begin{bmatrix} e^{i\omega t/2}/\sqrt{2} \\ e^{-i\omega t/2}/\sqrt{2} \end{bmatrix} = \frac{\hbar}{2} i (e^{i\omega t} - e^{-i\omega t}) = -\frac{\hbar}{2} \sin \omega t \end{aligned}$$

This looks right. At $t = 0$, the state is a pure $|+\hat{x}\rangle$, so $\langle S_y \rangle = 0$. The expectation value precesses (apparently in the clockwise direction) about the $+z$ axis. (This will be clear when we study rotations.)

(4) In this case, the Hamiltonian is

$$H = -\frac{q}{mc} \vec{\mathbf{S}} \cdot \vec{\mathbf{B}} = +\omega S_z \quad \text{with} \quad \omega \equiv \frac{eB}{mc} \quad \text{so} \quad U(t) = \exp\left(-\frac{iHt}{\hbar}\right) = \exp\left(\frac{-i\omega S_z t}{\hbar}\right)$$

where $q = -e$ is the charge on the electron. The initial state is, from HW 1 with $\phi = 0$,

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

The state of the particle at time t is just given by

$$\begin{aligned} |\alpha; t\rangle &= U(t)|+\hat{\mathbf{n}}\rangle = \exp\left(-\frac{i\omega S_z t}{\hbar}\right) \left[\cos\frac{\theta}{2}|+\hat{\mathbf{z}}\rangle + \sin\frac{\theta}{2}|-\hat{\mathbf{z}}\rangle \right] \\ &= e^{-i\omega t/2} \cos\frac{\theta}{2}|+\hat{\mathbf{z}}\rangle + e^{i\omega t/2} \sin\frac{\theta}{2}|-\hat{\mathbf{z}}\rangle \end{aligned}$$

The probability to find the electron in the $|+\hat{\mathbf{x}}\rangle$ state is

$$\begin{aligned} |\langle+\hat{\mathbf{x}}|\alpha; t\rangle|^2 &= \left| \left[\frac{1}{\sqrt{2}}\langle+\hat{\mathbf{z}}| + \frac{1}{\sqrt{2}}\langle-\hat{\mathbf{z}}| \right] \left[e^{-i\omega t/2} \cos\frac{\theta}{2}|+\hat{\mathbf{z}}\rangle + e^{i\omega t/2} \sin\frac{\theta}{2}|-\hat{\mathbf{z}}\rangle \right] \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} e^{-i\omega t/2} \cos\frac{\theta}{2} + \frac{1}{\sqrt{2}} e^{i\omega t/2} \sin\frac{\theta}{2} \right|^2 = \frac{1}{2} \left| \cos\frac{\theta}{2} + e^{i\omega t} \sin\frac{\theta}{2} \right|^2 \\ &= \frac{1}{2} \left[\cos\frac{\theta}{2} + e^{i\omega t} \sin\frac{\theta}{2} \right] \left[\cos\frac{\theta}{2} + e^{-i\omega t} \sin\frac{\theta}{2} \right] \\ &= \frac{1}{2} \left[1 + \cos\frac{\theta}{2} \sin\frac{\theta}{2} (e^{i\omega t} + e^{-i\omega t}) \right] = \frac{1}{2} [1 + \sin\theta \cos\omega t] \end{aligned}$$

In order to find $\langle S_x \rangle = \langle \alpha; t | S_x | \alpha; t \rangle$, first find

$$\begin{aligned} S_x |\alpha; t\rangle &= \frac{\hbar}{2} [|+\hat{\mathbf{z}}\rangle \langle-\hat{\mathbf{z}}| + |-\hat{\mathbf{z}}\rangle \langle+\hat{\mathbf{z}}|] \left[e^{-i\omega t/2} \cos\frac{\theta}{2}|+\hat{\mathbf{z}}\rangle + e^{i\omega t/2} \sin\frac{\theta}{2}|-\hat{\mathbf{z}}\rangle \right] \\ &= \frac{\hbar}{2} \left[e^{i\omega t/2} \sin\frac{\theta}{2}|+\hat{\mathbf{z}}\rangle + e^{-i\omega t/2} \cos\frac{\theta}{2}|-\hat{\mathbf{z}}\rangle \right] \end{aligned}$$

Therefore

$$\begin{aligned} \langle \alpha; t | S_x | \alpha; t \rangle &= \left[e^{i\omega t/2} \cos\frac{\theta}{2} \langle+\hat{\mathbf{z}}| + e^{-i\omega t/2} \sin\frac{\theta}{2} \langle-\hat{\mathbf{z}}| \right] \frac{\hbar}{2} \left[e^{i\omega t/2} \sin\frac{\theta}{2}|+\hat{\mathbf{z}}\rangle + e^{-i\omega t/2} \cos\frac{\theta}{2}|-\hat{\mathbf{z}}\rangle \right] \\ &= \frac{\hbar}{2} \left[e^{i\omega t} \cos\frac{\theta}{2} \sin\frac{\theta}{2} + e^{-i\omega t} \sin\frac{\theta}{2} \cos\frac{\theta}{2} \right] = \frac{\hbar}{2} \sin\theta \cos\omega t \end{aligned}$$

For $\theta = 0$, we are in the $|+\hat{\mathbf{z}}\rangle$ state, so it makes sense that the probability of measuring the $|+\hat{\mathbf{x}}\rangle$ state is always $1/2$, and the expectation value would be 0. For $\theta = \pi/2$, we are in the $|\pm\hat{\mathbf{x}}\rangle$ state (to start) so the probability starts out at unity and reduces to zero at $t = \pi/\omega = T/2$ when it rotates into the $|-\hat{\mathbf{x}}\rangle$ state. In this case, the expectation value oscillates between $\pm\hbar/2$ with period $2\pi/\omega$. It's all good.

(5) The time-evolved state is

$$|\nu_e; t\rangle = e^{-iHt/\hbar}|\nu_e\rangle = e^{-iHt/\hbar}[\cos\theta|\nu_1\rangle - \sin\theta|\nu_2\rangle] = e^{-iE_1t/\hbar}\cos\theta|\nu_1\rangle - e^{-iE_2t/\hbar}\sin\theta|\nu_2\rangle$$

Therefore the survival probability is

$$\begin{aligned} P(\nu_e \rightarrow \nu_e) &= |\langle\nu_e|\nu_e; t\rangle|^2 \\ &= |\cos\theta\langle\nu_1| - \sin\theta\langle\nu_2| [e^{-iE_1t/\hbar}\cos\theta|\nu_1\rangle - e^{-iE_2t/\hbar}\sin\theta|\nu_2\rangle]|^2 \\ &= |e^{-iE_1t/\hbar}\cos^2\theta + e^{-iE_2t/\hbar}\sin^2\theta|^2 \\ &= \cos^4\theta + \sin^4\theta + 2\cos^2\theta\sin^2\theta\cos\left[\frac{(E_1 - E_2)t}{\hbar}\right] \end{aligned}$$

Now make use of the momentum being much higher than the masses to write

$$\begin{aligned} E_2 - E_1 &= pc\left(1 + \frac{m_1^2c^2}{p^2}\right)^{1/2} - pc\left(1 + \frac{m_2^2c^2}{p^2}\right)^{1/2} \\ &\approx pc\left(1 + \frac{m_1^2c^2}{2p^2}\right) - pc\left(1 + \frac{m_2^2c^2}{2p^2}\right) = \frac{c^3}{2p}\Delta m^2 \\ \text{so } \frac{(E_1 - E_2)t}{\hbar} &= \frac{c^3}{2p}\Delta m^2 \frac{L}{c} \frac{1}{\hbar} = \Delta m^2 c^4 \frac{L}{2E\hbar c} \equiv \mu \end{aligned}$$

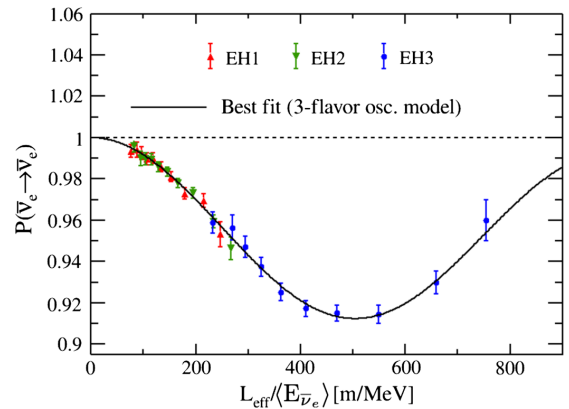
Now it is just some algebra with trigonometric functions. We have

$$\begin{aligned} P(\nu_e \rightarrow \nu_e) &= \cos^4\theta + \sin^4\theta + 2\cos^2\theta\sin^2\theta\cos\mu \\ &= \cos^2\theta(1 - \sin^2\theta) + \sin^2\theta(1 - \cos^2\theta) + 2\cos^2\theta\sin^2\theta\cos\mu \\ &= 1 - 2\sin^2\theta\cos^2\theta(1 - \cos\mu) = 1 - \sin^2 2\theta \sin(\mu/2) \end{aligned}$$

which is the formula we were asked to prove.

The figure is shown here. The difference between unity and the curve at the bottom of the trough gives $\sin^2 2\theta \approx 0.08$, in good agreement with the value 0.0851 ± 0.0024 given in the paper. The position of the trough corresponds to $\mu/2 = \pi/2$ when $L/E \approx 500$ m/MeV, so

$$\Delta m^2 c^4 \frac{L}{2E\hbar c} = \pi$$



Writing $\hbar c = 200$ MeV · fm = 2×10^{-7} eV · m and $L/E = 5 \times 10^{-4}$ m/eV we get

$$\Delta m^2 c^4 = 2\pi \frac{2 \times 10^{-7}}{5 \times 10^{-4}} \text{ eV}^2 = 2.51 \times 10^{-3} \text{ eV}^2$$

which also agrees well with the published value $(2.466 \pm 0.060) \times 10^{-3} \text{ eV}^2$.

PHYS3701 Intro Quantum Mechanics I HW#4 Due 13 Feb 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) In class, we showed that the time dependence of the expectation value for an observable A , where A itself is independent of time, is given by

$$\frac{d}{dt}\langle A \rangle = \frac{1}{i\hbar}\langle a; t|[A, H]|\alpha; t \rangle$$

Show that this holds for Problem 3 of Homework 3, namely $\langle S_y \rangle$ for a spin-1/2 particle with charge q in a static magnetic field $\vec{B} = B\hat{z}$, initially in the state $|+\hat{x}\rangle$.

(2) Prove the second of “Hamilton’s Equations” for expectation values, namely

$$\frac{d}{dt}\langle p_x \rangle = \left\langle -\frac{dV}{dx} \right\rangle$$

- (a) First prove that $[x^n, p_x] = i\hbar n x^{n-1}$ for an integer n , by first showing that it is true for $n = 1$, and then showing that if it is true for n , then it is true for $n + 1$.
- (b) Next, using a Taylor expansion for $F(x)$, show that $[F(x), p_x] = i\hbar \partial F / \partial x$.
- (c) Finally, derive the desired result using the Hamiltonian $H = p_x^2 / 2m + V(x)$.

(3) In this problem you will derive the Heisenberg Uncertainty Principle $\Delta x \Delta p_x \geq \hbar/2$, but using proper quantum mechanical notation and formalism.

- (a) Show that $\langle (\Delta A)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$, where, for an observable A , we define the operator $\Delta A = A - \langle A \rangle$. What does $\langle (\Delta A)^2 \rangle^{1/2}$ remind you of?
- (b) Prove the Schwarz (aka “triangle”) inequality $\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2$ where $|\alpha\rangle$ and $|\beta\rangle$ are arbitrary states. Start by taking the inner product of $|\alpha\rangle + \lambda|\beta\rangle$ with itself and invoke the positivity postulate. Then make a wise choice for λ .
- (c) An *anti*-Hermitian operator C is one for which $C^\dagger = -C$. Show that the product XY of any two *Hermitian* operators X and Y can be written as the sum of Hermitian and anti-Hermitian operators. Then prove that the expectation value of any Hermitian (anti-Hermitian) operator is purely real (imaginary).
- (d) Apply the above ideas to states $|\alpha\rangle = \Delta A |\gamma\rangle$ and $|\beta\rangle = \Delta B |\gamma\rangle$ to prove that

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} |\langle [A, B] \rangle|^2$$

and thereby derive the Heisenberg Uncertainty Principle.

(4) Given a state $|\alpha\rangle$, find the “momentum space wave function” $\phi_\alpha(p'_x) = \langle p'_x | \alpha \rangle$ in terms of the wave function $\psi_\alpha(x')$ and an integral. What is this called? (You’ve seen it before!)

(5) Two states $|\alpha\rangle$ and $|\beta\rangle$ are related by $|\beta\rangle = e^{ip_0 x / \hbar} |\alpha\rangle$ where x is the position operator and p_0 is a constant. Using a subscript to indicate the state in which the expectation value is calculated, show that

$$\langle x \rangle_\beta = \langle x \rangle_\alpha \quad \text{and} \quad \langle p_x \rangle_\beta = \langle p_x \rangle_\alpha + p_0$$

(1) Problem 3 of Homework 3 found that

$$|\alpha; t\rangle = \frac{e^{i\omega t/2}}{\sqrt{2}} |+\hat{z}\rangle + \frac{e^{-i\omega t/2}}{\sqrt{2}} |-\hat{z}\rangle \quad \text{and} \quad \langle S_y \rangle = -\frac{\hbar}{2} \sin \omega t$$

The Hamiltonian in this case is $H = -\omega S_z$, so we are asked to show that

$$\frac{d}{dt} \langle S_y \rangle = -\frac{\hbar\omega}{2} \cos \omega t = -\frac{\omega}{i\hbar} \langle \alpha; t | [S_y, S_z] | \alpha; t \rangle$$

It is probably simplest to calculate the commutator with matrices, that is

$$\begin{aligned} [S_y, S_z] &\doteq \frac{\hbar^2}{4} \left\{ \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \right\} \\ &= \frac{\hbar^2}{4} \left\{ \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix} \right\} = \frac{i\hbar^2}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \doteq i\hbar S_x \end{aligned}$$

To get the expectation value, we just follow the example of the solution to Problem 3 of Homework 3, but switching from S_y to S_x , that is

$$\begin{aligned} -\frac{\omega}{i\hbar} \langle \alpha; t | [S_y, S_z] | \alpha; t \rangle &= -\omega \langle \alpha; t | S_x | \alpha; t \rangle \\ &= -\omega \begin{bmatrix} e^{-i\omega t/2}/\sqrt{2} & e^{i\omega t/2}/\sqrt{2} \end{bmatrix} \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} e^{i\omega t/2}/\sqrt{2} \\ e^{-i\omega t/2}/\sqrt{2} \end{bmatrix} \\ &= -\frac{\hbar\omega}{2} \begin{bmatrix} e^{i\omega t/2}/\sqrt{2} & e^{-i\omega t/2}/\sqrt{2} \end{bmatrix} \begin{bmatrix} e^{i\omega t/2}/\sqrt{2} \\ e^{-i\omega t/2}/\sqrt{2} \end{bmatrix} \\ &= -\frac{\hbar\omega}{2} \frac{1}{2} (e^{i\omega t} + e^{-i\omega t}) = -\frac{\hbar\omega}{2} \cos \omega t \end{aligned}$$

and, indeed, the two expressions are equal.

(2) I think the proof in (a) is called “proof by induction.” For $n = 1$, the statement is simply the canonical conjugation relation. We then have

$$\begin{aligned} [x^{n+1}, p_x] &= x^{n+1} p_x - p_x x^{n+1} = x^n (x p_x) - p_x x^{n+1} = x^n (i\hbar + p_x x) - p_x x^{n+1} \\ &= i\hbar x^n + x^n p_x x - p_x x^n x = i\hbar x^n + [x^n, p_x] x = i\hbar x^n + i\hbar n x^{n-1} x \\ &= i\hbar (n+1) x^n \end{aligned}$$

and we are done. Part (b) follows easily, that is

$$[F(x), p_x] = \left[\sum_{n=0}^{\infty} a_n x^n, p_x \right] = \sum_{n=0}^{\infty} a_n [x^n, p_x] = \sum_{n=0}^{\infty} i\hbar n a_n x^{n-1} = i\hbar \frac{\partial F}{\partial x}$$

Finally, noting that p_x of course commutes with itself,

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

(3) See Section 1.4.5 of MQM3e. Part (a) is simple, that is

$$\langle(\Delta A)^2\rangle = \langle(A - \langle A\rangle)^2\rangle = \langle A^2\rangle - 2\langle A\rangle\langle A\rangle + \langle A\rangle^2 = \langle A^2\rangle - \langle A\rangle^2$$

For some data sample, we would call this the “variance”, and $\langle(\Delta A)^2\rangle^{1/2} \equiv \sigma$ would be the “standard deviation.” Now for Part (a), just follow the instructions to get

$$\langle(\alpha| + \lambda^*\langle\beta|)(|\alpha\rangle + \lambda|\beta\rangle)\rangle = \langle\alpha|\alpha\rangle + \lambda\langle\alpha|\beta\rangle + \lambda^*\langle\beta|\alpha\rangle + |\lambda|^2\langle\beta|\beta\rangle \geq 0$$

We want to end up with a factor $\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$ so it looks like we want λ to have $\langle\beta|\beta\rangle$ in the denominator. Writing $\lambda = a/\langle\beta|\beta\rangle$ and multiplying through by $\langle\beta|\beta\rangle$ gives us

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle + a\langle\alpha|\beta\rangle + a^*\langle\beta|\alpha\rangle + |a|^2 \geq 0$$

This clearly suggests that we put $a = -\langle\beta|\alpha\rangle$, so

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq \langle\beta|\alpha\rangle\langle\alpha|\beta\rangle + \langle\beta|\alpha\rangle^*\langle\beta|\alpha\rangle - |\langle\beta|\alpha\rangle|^2 = |\langle\alpha|\beta\rangle|^2 + |\langle\alpha|\beta\rangle|^2 - |\langle\alpha|\beta\rangle|^2 = |\langle\alpha|\beta\rangle|^2$$

and we’re done. For Part (c), it is more or less obvious that

$$XY = \frac{1}{2}(XY + YX) + \frac{1}{2}(XY - YX) \equiv \frac{1}{2}\{X, Y\} + \frac{1}{2}[X, Y] \equiv A + C$$

where $A^\dagger = A$ and $C^\dagger = -C$. Now $\langle\alpha|A|\beta\rangle = \langle\beta|A^\dagger|\alpha\rangle^* = \langle\beta|A|\alpha\rangle^*$ so $\langle\alpha|A|\alpha\rangle = \langle\alpha|A|\alpha\rangle^*$ which proves that the expectation value of a Hermitian operator is purely real. Similarly, $\langle\alpha|C|\alpha\rangle = -\langle\alpha|C|\alpha\rangle^*$ which proves that the expectation value of an anti-Hermitian operator is purely imaginary. Putting this together for Part (d) gives us

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq |\langle\Delta A\Delta B\rangle|^2 = \left|\frac{1}{2}\langle\{\Delta A, \Delta B\}\rangle + \frac{1}{2}\langle[\Delta A, \Delta B]\rangle\right|^2$$

The first time inside the square on the right is purely real and the second is purely imaginary, so the square of the sum is just the sum of the squares, where both terms are strictly positive. Therefore

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[\Delta A, \Delta B]\rangle|^2 = \frac{1}{4}|\langle[A, B]\rangle|^2$$

where the other pieces from ΔA and ΔB cancel in the commutator. The canonical commutation relation is $[x, p_x] = i\hbar$, so

$$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle \geq \frac{1}{4}|\langle[x, p_x]\rangle|^2 = \frac{\hbar^2}{4} \quad \text{or} \quad \langle(\Delta x)^2\rangle^{1/2}\langle(\Delta p_x)^2\rangle^{1/2} \geq \frac{\hbar}{2}$$

(4) Just insert a complete set of position basis states to get

$$\phi_\alpha(p'_x) = \langle p'_x | \alpha \rangle = \int_{-\infty}^{\infty} \langle p'_x | x' \rangle \langle x' | \alpha \rangle dx' = \int_{-\infty}^{\infty} \langle p'_x | x' \rangle \psi_\alpha(x') dx'$$

From class, we know that $\langle p'_x | x' \rangle = \exp(-ip'_x x' / \hbar) / \sqrt{2\pi\hbar}$, so

$$\phi_\alpha(p'_x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ip'_x x' / \hbar} \psi_\alpha(x') dx'$$

This is just a Fourier transform, easy to see if we write $k = p_x / \hbar$.

(5) The first part is simple, since x commutes with $\exp(ip_0 x / \hbar)$.

$$\langle x \rangle_\beta = \langle \beta | x | \beta \rangle = \langle \alpha | e^{-ip_0 x / \hbar} x e^{ip_0 x / \hbar} | \alpha \rangle = \langle \alpha | e^{-ip_0 x / \hbar} e^{ip_0 x / \hbar} x | \alpha \rangle = \langle \alpha | x | \alpha \rangle = \langle x \rangle_\alpha$$

For the second part, we have to know how to switch the order of $\exp(ip_0 x / \hbar)$ and p_x , but for this we can make use of a result derived in Problem 2, namely

$$[\exp(ip_0 x / \hbar), p_x] = i\hbar \frac{\partial}{\partial x} \exp(ip_0 x / \hbar) = -p_0 \exp(ip_0 x / \hbar)$$

We can now calculate

$$\begin{aligned} \langle p_x \rangle_\beta = \langle \beta | p_x | \beta \rangle &= \langle \alpha | e^{-ip_0 x / \hbar} p_x e^{ip_0 x / \hbar} | \alpha \rangle \\ &= \langle \alpha | e^{-ip_0 x / \hbar} (e^{ip_0 x / \hbar} p_x + p_0 e^{ip_0 x / \hbar}) | \alpha \rangle \\ &= \langle \alpha | p_x | \alpha \rangle + p_0 = \langle p_x \rangle_\alpha + p_0 \end{aligned}$$

PHYS3701 Intro Quantum Mechanics I HW#5 Due 20 Feb 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) A particle of mass m is initially in the Gaussian wave packet

$$\psi_{\alpha}(x) = \frac{1}{\sigma^{1/2}\pi^{1/4}}e^{-x^2/2\sigma^2}$$

- Prove that this wave function is properly normalized.
- Show that the uncertainty $\Delta x = \sigma/\sqrt{2}$.
- Find the uncertainty Δp_x and compare $\Delta x\Delta p_x$ to the Heisenberg uncertainty principle.

It would be useful to review the material on Gaussian integrals in the Concepts textbook.

(2) The height of a vertically bouncing ball is quantized. Numerically solve the Schrödinger equation for $V(x) = mgx$ with $\psi(0) = 0$ and adjust the lowest energy eigenvalue until you see $\psi \rightarrow 0$ at large x . You can choose whatever you like for $\psi'(0)$. It is best to write the differential equation in terms of dimensionless $y = x/x_0$ and $\epsilon = E/mgx_0$, where $x_0 = (\hbar^2/m^2g)^{1/3}$. (You should find that ϵ is between one and two.) Compare your answer to the experiment described in V. V. Nesvizhevsky, *et al.*, Phys. Rev. D 67(2003)102002.

(3) A particle of mass m is bound in an infinite one-dimensional square well. If the quantum mechanical state of the particle is initially given by an equal mixture of the ground and first excited states, find the probability as a function of time that the particle is found in the left half of the well. (You can assume that the coefficients of the mixture are relatively real.) Plot this probability for as a function of time for one period corresponding the frequency of the ground state component, that is for $0 \leq t \leq T$ where $T = 2\pi/\omega$ with $E_1 = \hbar\omega$. Make an animation showing how the probability density $\rho(x, t) = \Psi^*(x, t)\Psi(x, t)$ changes over time, and convince yourself that your animation agrees with your plot.

(4) A particle of mass m is bound by a potential energy function $V(x) = -(\hbar^2/2m)(\lambda/a)\delta(x)$ where a has the dimensions of length. Show that there is only one bound state, and find the energy eigenvalue and (normalized) eigenfunction. You will find it useful to integrate the Schrödinger equation over the range $-\epsilon \leq x \leq +\epsilon$ and then let $\epsilon \rightarrow 0$.

(5) A particle of mass m and energy $E > 0$ is incident on a potential energy well given by $V(x) = -(\hbar^2/2m)(\lambda/a)\delta(x)$ where a has the dimensions of length. Calculate the reflection and transmission coefficients, and show that they add up to unity, and confirm that you get the answers you expect for $\lambda \rightarrow 0$ and $\lambda \rightarrow \infty$.

(1) First recall two results from Concepts Section 1.5.6:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \quad \text{and} \quad \int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a^3}}$$

To check that the wave function is properly normalized, we write

$$\int_{-\infty}^{\infty} \psi^* \psi dx = \int_{-\infty}^{\infty} \frac{1}{\sigma\pi^{1/2}} e^{-x^2/\sigma^2} = \frac{1}{\sigma\pi^{1/2}} \sigma\sqrt{\pi} = 1$$

We know that $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$, but $\langle x \rangle = \int \psi^* x \psi dx = 0$ since $\psi^* \psi = \psi^2$ is an even function of x . Therefore

$$(\Delta x)^2 = \langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi dx = \int_{-\infty}^{\infty} x^2 \frac{1}{\sigma\pi^{1/2}} e^{-x^2/\sigma^2} dx = \frac{1}{\sigma\pi^{1/2}} \frac{1}{2} \sqrt{\pi\sigma^6} = \frac{\sigma^2}{2}$$

and so $\Delta x = \sigma/\sqrt{2}$. We can find Δp_x directly from the wave function, or also by using the momentum space wave function. Using the former, and noting again that $\langle p_x \rangle = 0$, we have

$$(\Delta p_x)^2 = \langle \alpha | p_x^2 | \alpha \rangle = \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar}{i} \frac{d}{dx} \right) \left(\frac{\hbar}{i} \frac{d}{dx} \right) \psi dx = -\hbar^2 \int_{-\infty}^{\infty} \psi^* \frac{d^2 \psi}{dx^2} dx$$

Now we calculate

$$\frac{d^2 \psi}{dx^2} = \frac{1}{\sigma^{1/2} \pi^{1/4}} \frac{d}{dx} \left[-\frac{x}{\sigma^2} e^{-x^2/2\sigma^2} \right] = \frac{1}{\sigma^{1/2} \pi^{1/4}} \left[\frac{x^2}{\sigma^4} - \frac{1}{\sigma^2} \right] e^{-x^2/2\sigma^2}$$

Therefore we get

$$(\Delta p_x)^2 = -\hbar^2 \frac{1}{\sigma\pi^{1/2}} \int_{-\infty}^{\infty} \left[\frac{x^2}{\sigma^4} - \frac{1}{\sigma^2} \right] e^{-x^2/\sigma^2} dx = -\hbar^2 \frac{1}{\sigma\pi^{1/2}} \left[\frac{1}{\sigma^4} \frac{1}{2} \sqrt{\pi\sigma^6} - \frac{1}{\sigma^2} \sigma\sqrt{\pi} \right] = \frac{\hbar^2}{2\sigma^2}$$

so $\Delta p_x = \hbar/\sigma\sqrt{2}$ and $\Delta x \Delta p_x = \hbar/2$, the minimum allowed by the uncertainty principle.

(2) The time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + mgx \psi = E \psi$$

Making the recommended substitutions gives

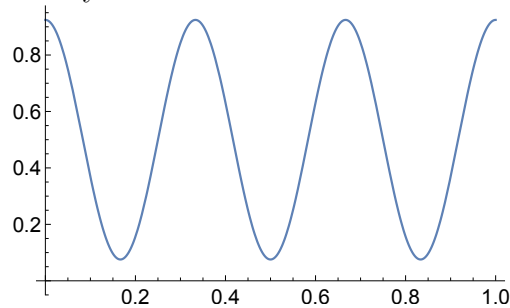
$$\begin{aligned} -\frac{\hbar^2}{2m} \left(\frac{m^2 g}{\hbar^2} \right)^{2/3} \frac{d^2 \psi}{dy^2} + mg \left(\frac{\hbar^2}{m^2 g} \right)^{1/3} y \psi &= mg \left(\frac{\hbar^2}{m^2 g} \right)^{1/3} \epsilon \psi \\ -\frac{\hbar^2}{2m^2 g} \left(\frac{\hbar^2}{m^2 g} \right)^{-2/3} \frac{d^2 \psi}{dy^2} + \left(\frac{\hbar^2}{m^2 g} \right)^{1/3} y \psi &= \left(\frac{\hbar^2}{m^2 g} \right)^{1/3} \epsilon \psi \\ \text{so} \quad \frac{d^2 \psi}{dy^2} + 2(\epsilon - y) \psi &= 0 \end{aligned}$$

See the MATHEMATICA notebook. With a little poking around, we find a solution for $\epsilon = 1.8557$ which translates into a height of about $14 \mu\text{m}$. This is in excellent agreement with Figure 5 of V. V. Nesvizhevsky, *et al.*, Phys. Rev. D 67(2003)102002, which shows that neutrons are not detected until they are allowed to bounce to at least this height.

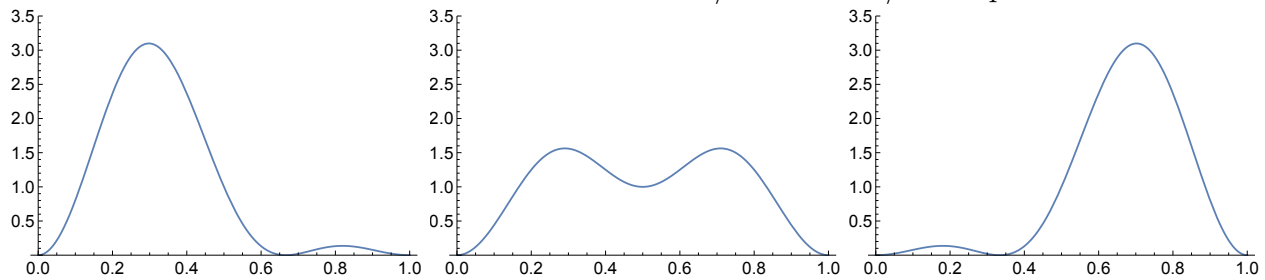
(3) See the MATHEMATICA notebook. The probability works out to be

$$\text{Prob}(0 \leq x \leq L/2) = \frac{4}{3\pi} \cos\left(\frac{3\pi^2 t \hbar}{2L^2 m}\right) + \frac{1}{2}$$

Here is the plot of the probability as a function of time:



Here are scenes from the animation $t = 0$ and $t = 1/4$ and $t = 1/2$ of a period:



(4) The Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \frac{\hbar^2}{2ma} \delta(x)\psi(x) = E\psi(x) \equiv -\frac{\hbar^2\kappa^2}{2m}\psi(x) \quad \text{or} \quad \frac{d^2\psi}{dx^2} + \frac{\lambda}{a}\delta(x)\psi(x) = \kappa^2\psi(x)$$

Integrating this over $-\epsilon \leq x \leq +\epsilon$ gives

$$\frac{d\psi}{dx}\Big|_{\epsilon} - \frac{d\psi}{dx}\Big|_{-\epsilon} + \frac{\lambda}{a}\psi(0) = \kappa^2 [\psi(\epsilon) - \psi(-\epsilon)] \rightarrow 0 \quad \text{for} \quad \epsilon \rightarrow 0$$

which ends up being a condition on the left and right slopes at $x = 0$ in terms of $\psi(0)$. Now for $x \neq 0$, we have

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi(x) \quad \text{so} \quad \psi(x) = \psi(0)e^{\pm\kappa x}$$

which means that $\psi(x) = \psi(0)e^{-\kappa x}$ for $x > 0$, and $\psi(x) = \psi(0)e^{+\kappa x}$ for $x < 0$. Therefore

$$-\kappa\psi(0) - \kappa\psi(0) + \frac{\lambda}{a}\psi(0) = 0 \quad \text{so} \quad \kappa = \frac{\lambda}{2a} \quad \text{and} \quad E = -\frac{\hbar^2\lambda^2}{8ma^2}$$

is the energy eigenvalue. To find $\psi(0)$ we just need to normalize, which means

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x) dx = 2\psi^2(0) \int_0^{\infty} e^{-2\kappa x} dx = 2\psi^2(0) \frac{1}{2\kappa} = 1 \quad \text{so} \quad \psi(0) = \sqrt{\kappa} = \sqrt{\frac{\lambda}{2a}}$$

(5) Proceed in standard fashion with

$$\psi(x < 0) = Ae^{ikx} + Be^{-ikx} \quad \text{and} \quad \psi(x > 0) = Ce^{ikx} \quad \text{where} \quad E = \frac{\hbar^2 k^2}{2m}$$

Continuity at $x = 0$ implies that $A + B = C$. Integrating across $x = 0$, exactly the same as we did in Problem 4, gives us

$$ikC - (ikA - ikB) + \frac{\lambda}{a}C = 0$$

The two equations for B/A and C/A are

$$\frac{C}{A} = 1 + \frac{B}{A} \quad \text{and} \quad \frac{C}{A} \left(1 + \frac{\lambda}{ika}\right) = 1 - \frac{B}{A}$$

The transmission coefficient is therefore

$$T = \left|\frac{C}{A}\right|^2 = \left|\frac{2}{2 + \lambda/ika}\right|^2 = \frac{4k^2 a^2}{4k^2 a^2 + \lambda^2}$$

This is clearly right for $\lambda \rightarrow 0$, and I guess it is reasonable that nothing gets through an infinitely deep δ -function potential. The reflection coefficient is

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{C}{A} - 1\right|^2 = \left|\frac{-\lambda/ika}{2 + \lambda/ika}\right|^2 = \frac{\lambda^2}{4k^2 a^2 + \lambda^2}$$

which again behaves as you'd expect as $\lambda \rightarrow 0$. It is also trivial to see that $R + T = 1$.

PHYS3701 Intro Quantum Mechanics I HW#6 Due 26 Feb 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) A particle of mass m is bound in a one-dimensional finite square well of height V_0 . Assume that the well extends over the range $-a \leq x \leq a$. Remember that the ground (first excited) state will be even (odd) parity.

- (a) Show that there will always be a solution for a ground state eigenvalue, but there may not be a solution for any other states if V_0 is too small.
- (b) Find the energy eigenvalues and plot their wave functions for the ground and first excited states assuming that $V_0 = 1.2(\hbar^2\pi^2/8ma^2)$. You will need to numerically solve two transcendental equations, one for the each of the two states. (*Hint:* In addition to matching boundary conditions, you can easily derive a formula for $(ka)^2 + (qa)^2$ where k and q are the wave numbers inside and outside the well.) Express the energy eigenvalues as a numerical factor times V_0 .

(2) Use induction to prove that the normalized states of the quantum harmonic oscillator are given by

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle$$

(3) Find $\langle x \rangle$ and $\langle p \rangle$ as a function of time for the initial state

$$|\alpha\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i\delta}}{\sqrt{2}}|1\rangle$$

where δ is a real number. Explain why this makes sense classically by taking the time derivative of $\langle x \rangle$ and showing that it has the expected relationship to $\langle p \rangle$, and interpret the physical meaning of the phase δ .

(4) The goal here is to find the harmonic oscillator normalized eigenfunction $\langle x|3\rangle$ using properties of the creation and annihilation operators.

- (a) Find the harmonic oscillator ground state wave function $\langle x|0\rangle$ by considering $\langle x|a|0\rangle$ and solving the resulting simple differential equation.
- (b) Now use the result from Problem (2) above to find $\langle x|3\rangle$ by building up from $\langle x|0\rangle$. Show that your result agrees with the result from solving the Schrödinger equation. Integrate to prove the normalization is correct. (The calculus in this part is messy. I suggest that you use MATHEMATICA.)

(5) Find Δx and Δp for the harmonic oscillator eigenstate $|n\rangle$ and compare the result to Heisenberg's uncertainty principle. Show that $n = 0$ yields the minimum possible result for the uncertainty product.

(1) We write the solutions to the Schrödinger equation for the ground state as

$$\begin{aligned} \psi(x) &= A \cos(kx) & \text{where} & \quad \frac{\hbar^2 k^2}{2m} = E & \text{for} & \quad -a \leq x \leq a \\ \text{with} \quad \psi(x) &= B e^{-qx} & \text{where} & \quad \frac{\hbar^2 q^2}{2m} = V_0 - E & \text{for} & \quad x > a \\ \text{and} \quad \psi(x) &= B e^{qx} & \text{where} & \quad \frac{\hbar^2 q^2}{2m} = V_0 - E & \text{for} & \quad x < -a \end{aligned}$$

Matching the wave function and its derivative at $x = a$ gives

$$A \cos(ka) = B e^{-qa} \quad \text{and} \quad -Ak \sin(ka) = -qB e^{-qa} \quad \text{so} \quad (ka) \tan(ka) = qa$$

The quantities ka and qa also need to satisfy

$$(ka)^2 + (qa)^2 = \frac{2ma^2}{\hbar^2} E + \frac{2ma^2}{\hbar^2} (V_0 - E) = \frac{2ma^2}{\hbar^2} V_0$$

These two equations will always find a solution for ka and qa because the first says that qa is a positive function of ka that increases from zero at $ka = 0$, and the second is just a circle around the origin, so those curves have to intersect. The first excited state will have $\psi(x) = A \sin(kx)$ inside the well, the same form for $x > a$, and the same form except $B \rightarrow -B$ for $x < 0$. Therefore

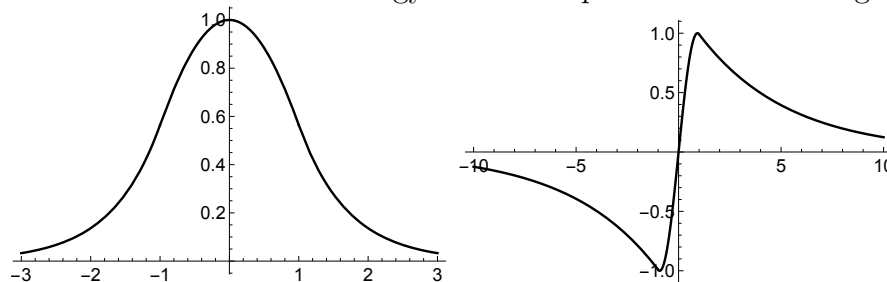
$$A \sin(ka) = B e^{-qa} \quad \text{and} \quad Ak \cos(ka) = -qB e^{-qa} \quad \text{so} \quad (ka) \cot(ka) = -qa$$

This will not necessarily have a solution if V_0 is too small. In that case, the radius of the circle is small enough that it will not intersect with $(ka) \cot(ka)$ which is positive for $ka < \pi/2$. In other words, for a shallow enough well, there will be only a ground state and no other bound states.

For this problem, the squared radius of the circle is $1.095 \times \pi/2$, so there will be a ground and excited state. See the MATHEMATICA notebook for details. The eigenvalues are

$$E_{\text{GS}} = \frac{\hbar^2 (ka)^2}{2ma^2} = \frac{\hbar^2}{2ma^2} (0.971)^2 = 0.319 V_0 \quad \text{and} \quad E_{1e} = \frac{\hbar^2}{2ma^2} (2.908)^2 = 0.982 V_0$$

Note how close the first excited state energy is to the top of the well. The eigenfunctions are



The closeness of the excited state energy to the top of the well leads to long tails on the wave function.

(2) This is trivially true for $n = 0$. (Recall that $0! = 1$ based on the definition the factorial through the Γ -function.) Therefore, assuming the relation is true for n ,

$$|n+1\rangle = \frac{1}{\sqrt{n+1}} a^\dagger |n\rangle = \frac{1}{\sqrt{n+1}} a^\dagger \left[\frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle \right] = \frac{1}{\sqrt{(n+1)!}} (a^\dagger)^{n+1} |0\rangle$$

which shows that it is true for $n+1$, so we are done.

(3) The time-dependent state is

$$|\alpha; t\rangle = e^{-iHt/\hbar} |\alpha\rangle = \frac{1}{\sqrt{2}} e^{-i\omega t/2} |0\rangle + \frac{e^{i\delta}}{\sqrt{2}} e^{-3i\omega t/2} |1\rangle = e^{-i\omega t/2} \left[\frac{1}{\sqrt{2}} |0\rangle + \frac{e^{-i(\omega t - \delta)}}{\sqrt{2}} |1\rangle \right]$$

Finding the expectation values is straightforward.

$$\begin{aligned} \langle x \rangle &= \left[\frac{1}{\sqrt{2}} \langle 0| + \frac{e^{i(\omega t - \delta)}}{\sqrt{2}} \langle 1| \right] \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) \left[\frac{1}{\sqrt{2}} |0\rangle + \frac{e^{-i(\omega t - \delta)}}{\sqrt{2}} |1\rangle \right] \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{2m\omega}} [\langle 0| + e^{i(\omega t - \delta)} \langle 1|] [e^{-i(\omega t - \delta)} |0\rangle + |1\rangle + e^{-i(\omega t - \delta)} \sqrt{2} |2\rangle] \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{2m\omega}} [e^{-i(\omega t - \delta)} + e^{i(\omega t - \delta)}] = \sqrt{\frac{\hbar}{2m\omega}} \cos(\omega t - \delta) \\ \langle p \rangle &= \left[\frac{1}{\sqrt{2}} \langle 0| + \frac{e^{i(\omega t - \delta)}}{\sqrt{2}} \langle 1| \right] i \sqrt{\frac{m\hbar\omega}{2}} (-a + a^\dagger) \left[\frac{1}{\sqrt{2}} |0\rangle + \frac{e^{-i(\omega t - \delta)}}{\sqrt{2}} |1\rangle \right] \\ &= \frac{1}{2} i \sqrt{\frac{m\hbar\omega}{2}} [\langle 0| + e^{i(\omega t - \delta)} \langle 1|] [-e^{-i(\omega t - \delta)} |0\rangle + |1\rangle + e^{-i(\omega t - \delta)} \sqrt{2} |2\rangle] \\ &= \frac{1}{2} i \sqrt{\frac{m\hbar\omega}{2}} [-e^{-i(\omega t - \delta)} + e^{i(\omega t - \delta)}] = -\sqrt{\frac{m\hbar\omega}{2}} \sin(\omega t - \delta) \end{aligned}$$

$$\text{so } \frac{d}{dt} \langle x \rangle = -\omega \sqrt{\frac{\hbar}{2m\omega}} \sin(\omega t - \delta) = \frac{1}{m} \langle p \rangle$$

which is just what you expect. Clearly δ is just the phase of the oscillation, that is δ/ω is the time lag from $t = 0$ to the peak of the oscillation.

(4) Defining $x_0 \equiv \sqrt{\hbar/m\omega}$, we know that

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{i}{m\omega} p \right) = \frac{1}{x_0 \sqrt{2}} \left(x - \frac{i}{\hbar} x_0^2 p \right)$$

It is simple to find $\langle x|0\rangle$ using the annihilation operator, that is

$$0 = \langle x|a|0\rangle = \langle x| \frac{1}{x_0 \sqrt{2}} \left(x + \frac{i}{\hbar} x_0^2 p \right) |0\rangle = \frac{1}{x_0 \sqrt{2}} \left(x \langle x|0\rangle + x_0^2 \frac{d}{dx} \langle x|0\rangle \right)$$

$$\text{so } \frac{d}{dx} \langle x|0\rangle = -\frac{1}{x_0^2} x \langle x|0\rangle \quad \text{and} \quad \langle x|0\rangle = N \exp\left(-\frac{x^2}{2x_0^2}\right)$$

$$\text{However } 1 = \langle 0|0\rangle = \int_{-\infty}^{\infty} \langle 0|x\rangle \langle x|0\rangle dx = \int_{-\infty}^{\infty} N^2 \exp\left(-\frac{x^2}{x_0^2}\right) dx = N^2 \pi^{1/2} x_0$$

$$\text{Therefore } \langle x|0\rangle = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left(-\frac{x^2}{2x_0^2}\right)$$

Now we also see that

$$\langle x|a^\dagger|\alpha\rangle = \langle x|\frac{1}{x_0\sqrt{2}}\left(x - \frac{i}{\hbar}x_0^2p\right)|\alpha\rangle = \frac{1}{x_0\sqrt{2}}\left[x - x_0^2\frac{d}{dx}\right]\langle x|\alpha\rangle$$

This makes it easy to see that, using the result from Problem (2),

$$\begin{aligned}\langle x|3\rangle &= \frac{1}{3!}\left(\frac{1}{2x_0^2}\right)^{3/2}\left[x - x_0^2\frac{d}{dx}\right]\left[x - x_0^2\frac{d}{dx}\right]\left[x - x_0^2\frac{d}{dx}\right]\langle x|0\rangle \\ &= \frac{1}{\pi^{1/4}x_0^{1/2}\sqrt{3}}\left[2\left(\frac{x}{x_0}\right)^3 - 3\frac{x}{x_0}\right]e^{-x^2/2x_0^2}\end{aligned}$$

where the derivatives were taken using MATHEMATICA in the accompanying notebook. This is indeed proportional to the Hermite polynomial $H_3(x) \propto 2x^2 - 3x$. The notebook shows that this wave function is properly normalized.

(5) Recall that we have

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \quad \text{and} \quad p = i\sqrt{\frac{m\hbar\omega}{2}}(-a + a^\dagger)$$

which makes it easy to see that $\langle n|x\rangle = \langle n|p\rangle = 0$ since the a and a^\dagger lower or raise n to a different (orthogonal) state. This makes sense, since the harmonic oscillator potential is symmetric. Therefore $\langle \Delta x \rangle^2 = \langle x^2 \rangle$ and $\langle \Delta p \rangle^2 = \langle p^2 \rangle$. Now we also have

$$x^2 = \frac{\hbar}{2m\omega}(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger) \quad \text{and} \quad p^2 = -\frac{m\hbar\omega}{2}(aa - aa^\dagger - a^\dagger a + a^\dagger a^\dagger)$$

The first and fourth terms in each of these two expressions contribute nothing to the expectation value because they raise or lower the quantum number by two. The second and third terms, however, do not change the quantum number. That is

$$aa^\dagger|n\rangle = a(\sqrt{n+1}|n+1\rangle) = (n+1)|n\rangle \quad \text{and} \quad a^\dagger a|n\rangle = a^\dagger(\sqrt{n}|n-1\rangle) = n|n\rangle$$

Therefore

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega}(2n+1) = \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right) \quad \text{and} \quad \langle p^2 \rangle = \frac{m\hbar\omega}{2}(2n+1) = m\hbar\omega\left(n + \frac{1}{2}\right)$$

and we end up with the result

$$\Delta x \Delta p = \langle x^2 \rangle^{1/2} \langle p^2 \rangle^{1/2} = \hbar\left(n + \frac{1}{2}\right)$$

which shows that the lowest eigenstate has the minimum possible uncertainty.

PHYS3701 Intro Quantum Mechanics I HW#7 Due 12 Mar 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) A particle of mass m is confined to a three dimensional “infinite box” of side length L in the region $0 \leq x, y, z \leq L$. Solve the time-independent Schrödinger equation to find the energy eigenvalues $E_{n_x, n_y, n_z} = \hbar^2 \vec{k}^2 / 2m$ and eigenfunctions $\psi_{n_x, n_y, n_z}(x, y, z)$ in terms of \hbar , m , L , and three positive integers n_x , n_y , and n_z . (This is easy to do using the technique of separation of variables and following what we did for the one-dimensional case.) Make a table of the lowest three energy levels, including their *degeneracy*, that is the number of combinations (n_x, n_y, n_z) that give the same energy.

(2) Write the operator S_x for a spin-1/2 system as linear combination of outer products of the $|\pm \hat{z}\rangle$ and show that its rotation $\exp(+i\phi S_z / \hbar) S_x \exp(-i\phi S_z / \hbar)$ is just what you expect. (This is written as the transformation of an operator. You might prefer to think of this in terms of the expectation value of the rotated operator in some state.)

(3) The three Pauli spin matrices are given by

$$\underline{\underline{\sigma_x}} \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \underline{\underline{\sigma_y}} \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \underline{\underline{\sigma_z}} \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

(a) Show that the representation of the spin operator \vec{S} in the $|\pm \hat{z}\rangle$ basis can be written as $\underline{\underline{S}} = (\hbar/2)\underline{\underline{\sigma}}$. (You are free to use results we have derived in class or on prior homework.)

(b) Prove that $(\underline{\underline{\sigma}} \cdot \underline{\underline{a}})^2 = |\underline{\underline{a}}|^2 \underline{\underline{1}}$ where the components of $\underline{\underline{a}}$ are real.

(c) Show that the rotation operator for spin-1/2 systems can be represented in the $|\pm \hat{z}\rangle$ basis as

$$\underline{\underline{D}}^{(1/2)}(\hat{n}, \phi) = \exp\left[-\frac{i}{\hbar} \underline{\underline{S}} \cdot \hat{n} \phi\right] = \underline{\underline{1}} \cos\left(\frac{\phi}{2}\right) - i \underline{\underline{\sigma}} \cdot \hat{n} \sin\left(\frac{\phi}{2}\right)$$

(d) Repeat Problem (2) above using matrix representations of the operators.

(4) Construct the matrix representations of the operators J_x and J_y for a spin-one system, in the J_z basis, spanned by the kets $|+\rangle \equiv |1, 1\rangle$, $|0\rangle \equiv |1, 0\rangle$, and $|-\rangle \equiv |1, -1\rangle$. Use these matrices to find the three analogous eigenstates for each of the two operators J_x and J_y in terms of $|+\rangle$, $|0\rangle$, and $|-\rangle$. You are welcome to use MATHEMATICA or some other app to find the eigenvalues and eigenstates after you’ve constructed the matrices.

(5) Using the fact that J_x , J_y , J_z , and $J_{\pm} \equiv J_x \pm iJ_y$ satisfy the usual angular-momentum commutation relations, prove that

$$\vec{J}^2 \equiv J_x^2 + J_y^2 + J_z^2 = J_z^2 + J_+ J_- - \hbar J_z$$

Using this result, or otherwise, derive the coefficient c_- that appears in $J_- |jm\rangle = c_- |j, m-1\rangle$.

(1) The Schrödinger equation inside the box is

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(x,y,z) = E\psi(x,y,z) = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)\psi(x,y,z)$$

Divide out the $\hbar^2/2m$, write $\psi(x,y,z) = X(x)Y(y)Z(z)$, divide through by $\psi(x,y,z)$, and rearrange to get

$$\left[\frac{1}{X}\frac{d^2X}{dx^2} - k_x^2\right] + \left[\frac{1}{Y}\frac{d^2Y}{dy^2} - k_y^2\right] + \left[\frac{1}{Z}\frac{d^2Z}{dz^2} - k_z^2\right] = 0$$

This has to be true for all x , y , and z , and the first term only depends on x , the second only on y , and the third on z . Therefore each of the three terms must equal zero. The wave function must vanish at the walls, so $\psi(0,0,0) = 0$, and $X(L) = 0 = Y(L) = Z(L)$. This all leads to sine functions and $k_xL = n_x\pi$, $k_yL = n_y\pi$, and $k_zL = n_z\pi$, where n_x , n_y , and n_z are all positive integers, and so on, all the same for the box in one dimension. The result is

$$\psi(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x\pi x}{L}\right) \sin\left(\frac{n_y\pi y}{L}\right) \sin\left(\frac{n_z\pi z}{L}\right) \quad \text{and} \quad E = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

The lowest energy is clearly for $n_x = n_y = n_z = 1$. Make any one of these equal to 2, and you get the second energy level, which therefore has a degeneracy of 3. Make two of them equal to 2 is not as high as making one of them equal to 3, so the first three energies are

n_x	n_y	n_z	E	Degeneracy
1	1	1	$3 \frac{\hbar^2\pi^2}{2mL^2}$	1
2	1	1	$6 \frac{\hbar^2\pi^2}{2mL^2}$	3
2	1	1		
2	1	1		
2	2	1	$9 \frac{\hbar^2\pi^2}{2mL^2}$	3
2	1	2		
1	2	2		

(2) Just do the work and you get exactly what you expect for an active rotation.

$$\begin{aligned} e^{i\phi S_z/\hbar} S_x e^{-i\phi S_z/\hbar} &= \frac{\hbar}{2} e^{i\phi S_z/\hbar} [|+\hat{z}\rangle \langle -\hat{z}| + |-\hat{z}\rangle \langle +\hat{z}|] e^{-i\phi S_z/\hbar} \\ &= \frac{\hbar}{2} [e^{i\phi/2} |+\hat{z}\rangle \langle -\hat{z}| e^{i\phi/2} + e^{-i\phi/2} |-\hat{z}\rangle \langle +\hat{z}| e^{i\phi/2}] \\ &= \frac{\hbar}{2} [(\cos\phi + i\sin\phi) |+\hat{z}\rangle \langle -\hat{z}| + (\cos\phi - i\sin\phi) |-\hat{z}\rangle \langle +\hat{z}|] \\ &= \cos\phi \frac{\hbar}{2} [|+\hat{z}\rangle \langle -\hat{z}| + |-\hat{z}\rangle \langle +\hat{z}|] - \sin\phi \frac{\hbar}{2} [-i |+\hat{z}\rangle \langle -\hat{z}| + i |-\hat{z}\rangle \langle +\hat{z}|] \\ &= \cos\phi S_x - \sin\phi S_y \\ \text{i.e. } {}_R\langle\alpha|S_x|\alpha\rangle_R &= \cos\phi \langle\alpha|S_x|\alpha\rangle - \sin\phi \langle\alpha|S_y|\alpha\rangle \end{aligned}$$

(3) It is trivial to show that this is the correct representation of the \vec{S} operator because we derived it in the past. Now

$$\begin{aligned} (\underline{\underline{\vec{\sigma}}} \cdot \vec{a})^2 &= \begin{bmatrix} a_z & a_x - ia_y \\ a_x + ia_y & -a_z \end{bmatrix} \begin{bmatrix} a_z & a_x - ia_y \\ a_x + ia_y & -a_z \end{bmatrix} \\ &= \begin{bmatrix} a_z^2 + a_x^2 + a_y^2 & 0 \\ 0 & a_x^2 + a_y^2 + a_z^2 \end{bmatrix} = |\vec{a}|^2 \underline{\underline{1}} \end{aligned}$$

This means that, for any non-negative integer m and some unit vector \hat{n} , $(\underline{\underline{\vec{\sigma}}} \cdot \hat{n})^m = \underline{\underline{1}}$ if m is even, and $(\underline{\underline{\vec{\sigma}}} \cdot \hat{n})^m = \underline{\underline{\vec{\sigma}}} \cdot \hat{n}$ if m is odd. These simple relationships imply that we can expand the matrix representation of the spin-1/2 rotation operator as a Taylor series of an exponential, because the matrices in the exponent all commute. That is

$$\begin{aligned} \underline{\underline{\mathcal{D}}}^{(1/2)}(\hat{n}, \phi) &= \exp \left[-\frac{i}{\hbar} \underline{\underline{\vec{S}}} \cdot \hat{n} \phi \right] = \exp \left[-i \frac{\phi}{2} (\underline{\underline{\vec{\sigma}}} \cdot \hat{n}) \right] \\ &= \underline{\underline{1}} \left[1 - \frac{1}{2!} \left(\frac{\phi}{2} \right)^2 + \frac{1}{4!} \left(\frac{\phi}{2} \right)^4 + \dots \right] \\ &\quad - i (\underline{\underline{\vec{\sigma}}} \cdot \hat{n}) \left[\left(\frac{\phi}{2} \right) - \frac{1}{3!} \left(\frac{\phi}{2} \right)^3 + \frac{1}{5!} \left(\frac{\phi}{2} \right)^5 + \dots \right] \\ &= \underline{\underline{1}} \cos \left(\frac{\phi}{2} \right) - i (\underline{\underline{\vec{\sigma}}} \cdot \hat{n}) \sin \left(\frac{\phi}{2} \right) \end{aligned}$$

Now Problem (2) is a rotation of S_x about the z -axis through an angle ϕ , so $\hat{n} = \hat{z}$ and the matrix representation of the rotation operator is

$$\underline{\underline{\mathcal{D}}}^{(1/2)}(\hat{z}, \phi) = \begin{bmatrix} \cos \frac{\phi}{2} - i \sin \frac{\phi}{2} & 0 \\ 0 & \cos \frac{\phi}{2} + i \sin \frac{\phi}{2} \end{bmatrix} = \begin{bmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{bmatrix}$$

and the rotated version of S_x is

$$\begin{aligned} \underline{\underline{\mathcal{D}}}^{(1/2)\dagger}(\hat{z}, \phi) \underline{\underline{S}}_x \underline{\underline{\mathcal{D}}}^{(1/2)}(\hat{z}, \phi) &= \frac{\hbar}{2} \begin{bmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{bmatrix} \\ &= \frac{\hbar}{2} \begin{bmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{bmatrix} \begin{bmatrix} 0 & e^{i\phi/2} \\ e^{-i\phi/2} & 0 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{bmatrix} \\ &= \cos \phi \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} - \sin \phi \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ &= \cos \phi \underline{\underline{S}}_x - \sin \phi \underline{\underline{S}}_y \end{aligned}$$

which is the same result we ended up with when we used operators in Problem (2).

(4) Finding the matrices is straightforward, using $J_x = (J_+ + J_-)/2$ and $J_y = (J_+ - J_-)/2i$, and applying

$$J_+ |j, m\rangle = \sqrt{(j-m)(j+m+1)} \hbar |j, m+1\rangle \quad \text{and} \quad J_- |j, m\rangle = \sqrt{(j+m)(j-m+1)} \hbar |j, m-1\rangle$$

to find the matrix elements of J_+ and J_- in the basis $|j, m\rangle = |1, 1\rangle, |1, 0\rangle, |1, -1\rangle$. The results, easily verified in other books or online, are

$$J_x \doteq \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad J_y \doteq \frac{\hbar}{i\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

See the accompanying MATHEMATICA notebook to find and normalize the eigenvectors. Find

$$|J_x; +\rangle = \frac{1}{2}|+\rangle + \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|-\rangle \quad |J_x; 0\rangle = -\frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle \quad |J_x; -\rangle = \frac{1}{2}|+\rangle - \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|-\rangle$$

$$|J_y; +\rangle = -\frac{1}{2}|+\rangle - \frac{i}{\sqrt{2}}|0\rangle + \frac{1}{2}|-\rangle \quad |J_y; 0\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle \quad |J_y; -\rangle = -\frac{1}{2}|+\rangle + \frac{i}{\sqrt{2}}|0\rangle + \frac{1}{2}|-\rangle$$

(5) It is easiest to first calculate

$$J_+J_- = (J_x + iJ_y)(J_x - iJ_y) = J_x^2 + J_y^2 - i[J_x, J_y] = J_x^2 + J_y^2 + \hbar J_z = \vec{J}^2 - J_z^2 + \hbar J_z$$

which immediately gives the result we were asked to prove. We then calculate

$$\begin{aligned} |c_-|^2 &= (\langle j, m | J_-^\dagger)(J_- | j, m \rangle) = \langle j, m | J_+ J_- | j, m \rangle = \langle j, m | (\vec{J}^2 - J_z^2 + \hbar J_z) | j, m \rangle \\ &= j(j+1)\hbar^2 - m^2\hbar^2 + m\hbar^2 = [j^2 - m^2 + j + m]\hbar^2 = [(j+m)(j-m+1)]\hbar^2 \end{aligned}$$

and, by convention, we choose $c_- = \hbar\sqrt{(j+m)(j-m+1)}$ to be real and positive.

PHYS3701 Intro Quantum Mechanics I HW#8 Due 19 Mar 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) Recall Problem (4) from Homework #1. Show that the state vector

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

can be obtained by rotating the state $|+\hat{\mathbf{z}}\rangle$ by an angle θ about the y -axis, and then by an angle ϕ about the z -axis. You can approach this using the rotation operators, or by using the matrix representation in the $|\pm\hat{\mathbf{z}}\rangle$ basis; I'm not sure which one is easiest.

(2) The spin-dependent part of the Hamiltonian for a hydrogen atom (proton plus electron) in an external magnetic field $\vec{B} = B\hat{\mathbf{z}}$ is

$$H = \frac{2A}{\hbar^2}\vec{S}_e \cdot \vec{S}_p + \omega S_{e_z}$$

where A is a positive constant and $\omega = geB/2mc$. Find the energy eigenvalues, and their expressions to lowest non-vanishing order for the cases (a) $A \gg \hbar\omega$ and (b) $A \ll \hbar\omega$. The calculations for the eigenvalues and their limits is not hard to do by hand, but you are welcome to resort to MATHEMATICA or some other app if you like.

(3) Consider a spin-3/2 system with the four states $|3/2, \pm 3/2\rangle$ and $|3/2, \pm 1/2\rangle$ made up from three spin-1/2 particles. Using the operator $S_z = S_{1_z} + S_{2_z} + S_{3_z}$, explain why we must have

$$\left|\frac{3}{2}, \frac{3}{2}\right\rangle = |+\hat{\mathbf{z}}, +\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle$$

Then use the operator S_- to similarly construct the other three states.

(4) Express the two electron spin-one state $|\alpha\rangle = |+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle$ in terms of the four states $|+\hat{\mathbf{x}}, +\hat{\mathbf{x}}\rangle$, $|+\hat{\mathbf{x}}, -\hat{\mathbf{x}}\rangle$, $|-\hat{\mathbf{x}}, +\hat{\mathbf{x}}\rangle$, and $|-\hat{\mathbf{x}}, -\hat{\mathbf{x}}\rangle$. Calculate the probability that a measurement of the x -direction spins of an electron pair in the state $|\alpha\rangle$ yields a result where the two electrons have spins in the opposite direction.

(5) Two spin-1/2 particles are emitted from the spin-one state $|+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle$ and move in opposite directions when they are measured independently by observers A and B who make measurements of the spins in the x -direction. Find the probabilities that A and B determine the two particles to be in the states $|1, +1\rangle_x$, $|1, 0\rangle_x$, and $|1, -1\rangle_x$.

(1) We need to calculate $\mathcal{D}(\hat{z}, \phi)\mathcal{D}(\hat{y}, \theta) |+\hat{z}\rangle$. If we did this with operators, then the z -rotation is easy, but the y -rotation would require us to write the first result in terms of the $|\pm\hat{y}\rangle$ basis, and that sounds tedious. Let's use the matrix representation, then. You find

$$\begin{aligned} & \mathcal{D}(\hat{z}, \phi)\mathcal{D}(\hat{y}, \theta) |+\hat{z}\rangle \\ \doteq & \begin{bmatrix} \cos(\phi/2) - i \sin(\phi/2) & 0 \\ 0 & \cos(\phi/2) + i \sin(\phi/2) \end{bmatrix} \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ = & \begin{bmatrix} \cos(\phi/2) - i \sin(\phi/2) & 0 \\ 0 & \cos(\phi/2) + i \sin(\phi/2) \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{bmatrix} \\ = & \begin{bmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{bmatrix} = e^{-i\phi/2} \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{bmatrix} = e^{-i\phi/2} \begin{bmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{bmatrix} \\ \doteq & e^{-i\phi/2} \left(\cos \frac{\theta}{2} |+\hat{z}\rangle + e^{i\phi} \sin \frac{\theta}{2} |-\hat{z}\rangle \right) \end{aligned}$$

with an additional phase factor in front. Note that if $\phi = 2\pi$, the phase factor is just the familiar factor of (-1) that we get when we do a full rotation of a spinor.

(2) Work in the same basis that we used in class, namely

$$|1\rangle = |+\hat{z}, +\hat{z}\rangle \quad |2\rangle = |+\hat{z}, -\hat{z}\rangle \quad |3\rangle = |-\hat{z}, +\hat{z}\rangle \quad |4\rangle = |-\hat{z}, -\hat{z}\rangle$$

We found the matrix elements of $2\vec{S}_e \cdot \vec{S}_p$ in this basis. The matrix elements of S_{e_z} are simple:

$$H \doteq \begin{bmatrix} A/2 + \hbar\omega/2 & 0 & 0 & 0 \\ 0 & -A/2 + \hbar\omega/2 & A & 0 \\ 0 & A & -A/2 - \hbar\omega/2 & 0 \\ 0 & 0 & 0 & A/2 - \hbar\omega/2 \end{bmatrix}$$

See the accompanying MATHEMATICA notebook to find the eigenvalues, and to take the two different limits. For the eigenvalues, you find

$$E = \left\{ \frac{A - \hbar\omega}{2}, \frac{A + \hbar\omega}{2}, \frac{1}{2} \left(-\sqrt{4A^2 + \hbar\omega^2} - A \right), \frac{1}{2} \left(\sqrt{4A^2 + \hbar\omega^2} - A \right) \right\}$$

It is important to note that this reduces to $A/2$ (three times) and $-3A/2$ for $\omega = 0$, which is what we got in class. For $\hbar\omega \ll A$, you find

$$E = \left\{ \frac{A}{2} - \frac{\hbar\omega}{2}, \frac{A}{2} + \frac{\hbar\omega}{2}, -\frac{3A}{2}, \frac{A}{2} \right\}$$

which shows that the triplet is split into three energy eigenvalues, the but singlet is unchanged. For $\hbar\omega \gg A$, you find

$$\left\{ \frac{A}{2} - \frac{\hbar\omega}{2}, \frac{A}{2} + \frac{\hbar\omega}{2}, -\frac{A}{2} - \frac{\hbar\omega}{2}, \frac{\hbar\omega}{2} - \frac{A}{2} \right\}$$

namely the normal result for spin-1/2 particles with some adjustment from the hyperfine interaction.

(3) The only combination of three $|\pm\hat{z}\rangle$ states that gives $3\hbar/2$ for S_z is the one where all three are $|+\hat{z}\rangle$, so the given state has to be the only combination. Now recall that

$$S_-|s, m\rangle = [s(s+1) - m(m-1)]^{1/2} \hbar|s, m-1\rangle$$

so
$$S_- \left| \frac{3}{2}, \frac{3}{2} \right\rangle = \left[\frac{3 \cdot 5}{2 \cdot 2} - \frac{3 \cdot 1}{2 \cdot 2} \right]^{1/2} \hbar \left| \frac{3}{2}, \frac{1}{2} \right\rangle = \sqrt{3} \hbar \left| \frac{3}{2}, \frac{1}{2} \right\rangle$$

and

$$(S_{1-} + S_{2-} + S_{3-})|+\hat{z}, +\hat{z}, +\hat{z}\rangle = \hbar(|-\hat{z}, +\hat{z}, +\hat{z}\rangle + |+\hat{z}, -\hat{z}, +\hat{z}\rangle + |+\hat{z}, +\hat{z}, -\hat{z}\rangle)$$

so
$$\left| \frac{3}{2}, \frac{1}{2} \right\rangle = \frac{1}{\sqrt{3}}|-\hat{z}, +\hat{z}, +\hat{z}\rangle + \frac{1}{\sqrt{3}}|+\hat{z}, -\hat{z}, +\hat{z}\rangle + \frac{1}{\sqrt{3}}|+\hat{z}, +\hat{z}, -\hat{z}\rangle$$

Now proceed in the same way for the next step down the ladder. First, we have

$$S_- \left| \frac{3}{2}, \frac{1}{2} \right\rangle = \left[\frac{3 \cdot 5}{2 \cdot 2} + \frac{1 \cdot 1}{2 \cdot 2} \right]^{1/2} \hbar \left| \frac{3}{2}, -\frac{1}{2} \right\rangle = 2\hbar \left| \frac{3}{2}, -\frac{1}{2} \right\rangle$$

Now we have to do $S_{1-} + S_{2-} + S_{3-}$ on three different combinations, but they are all similar. We know that $S_-|+\hat{z}\rangle = |-\hat{z}\rangle$, and $S_-|-\hat{z}\rangle = 0$, so, dropping the factor $\hbar/\sqrt{3}$,

$$\begin{aligned} & (S_{1-} + S_{2-} + S_{3-})(|-\hat{z}, +\hat{z}, +\hat{z}\rangle + |+\hat{z}, -\hat{z}, +\hat{z}\rangle + |+\hat{z}, +\hat{z}, -\hat{z}\rangle) \\ &= 0 + |-\hat{z}, -\hat{z}, +\hat{z}\rangle + |-\hat{z}, +\hat{z}, -\hat{z}\rangle \\ &+ |-\hat{z}, -\hat{z}, +\hat{z}\rangle + 0 + |+\hat{z}, -\hat{z}, -\hat{z}\rangle \\ &+ |-\hat{z}, +\hat{z}, -\hat{z}\rangle + |+\hat{z}, -\hat{z}, -\hat{z}\rangle + 0 = 2|-\hat{z}, -\hat{z}, +\hat{z}\rangle + 2|-\hat{z}, +\hat{z}, -\hat{z}\rangle + 2|+\hat{z}, -\hat{z}, -\hat{z}\rangle \end{aligned}$$

Therefore, remembering to put back the factor of $\hbar/\sqrt{3}$, we find

$$\left| \frac{3}{2}, -\frac{1}{2} \right\rangle = \frac{1}{\sqrt{3}}|-\hat{z}, -\hat{z}, +\hat{z}\rangle + \frac{1}{\sqrt{3}}|-\hat{z}, +\hat{z}, -\hat{z}\rangle + \frac{1}{\sqrt{3}}|+\hat{z}, -\hat{z}, -\hat{z}\rangle$$

which is what you would probably have expected. For the final down step, we have

$$S_- \left| \frac{3}{2}, -\frac{1}{2} \right\rangle = \left[\frac{3 \cdot 5}{2 \cdot 2} - \frac{1 \cdot 3}{2 \cdot 2} \right]^{1/2} \hbar \left| \frac{3}{2}, -\frac{3}{2} \right\rangle = \sqrt{3} \hbar \left| \frac{3}{2}, -\frac{3}{2} \right\rangle$$

and again holding back a factor of $\hbar/\sqrt{3}$, we calculate

$$\begin{aligned} & (S_{1-} + S_{2-} + S_{3-})(|-\hat{z}, -\hat{z}, +\hat{z}\rangle + |-\hat{z}, +\hat{z}, -\hat{z}\rangle + |+\hat{z}, -\hat{z}, -\hat{z}\rangle) \\ &= 2|-\hat{z}, -\hat{z}, -\hat{z}\rangle + 2|-\hat{z}, -\hat{z}, -\hat{z}\rangle + 2|-\hat{z}, -\hat{z}, -\hat{z}\rangle = 3|-\hat{z}, -\hat{z}, -\hat{z}\rangle \end{aligned}$$

Putting the factor of $\hbar/\sqrt{3}$ back, we have

$$\sqrt{3} \hbar \left| \frac{3}{2}, -\frac{3}{2} \right\rangle = \frac{\hbar}{\sqrt{3}} 3 |-\hat{z}, -\hat{z}, -\hat{z}\rangle \quad \text{or} \quad \left| \frac{3}{2}, -\frac{3}{2} \right\rangle = |-\hat{z}, -\hat{z}, -\hat{z}\rangle$$

which, of course, is exactly what you expect. Indeed, we could have started with this state, and climbed up the ladder instead of down, using S_+ instead of S_- .

(4) We start by noting that

$$|+\hat{z}\rangle = \frac{1}{\sqrt{2}}|+\hat{x}\rangle + \frac{1}{\sqrt{2}}|-\hat{x}\rangle \quad \text{and} \quad |-\hat{z}\rangle = \frac{1}{\sqrt{2}}|+\hat{x}\rangle - \frac{1}{\sqrt{2}}|-\hat{x}\rangle$$

It is now straightforward to write $|\alpha\rangle = |+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle$ in terms of x -kets:

$$\begin{aligned} |\alpha\rangle &= |+\hat{\mathbf{z}}\rangle \otimes |+\hat{\mathbf{z}}\rangle = \frac{1}{2} [|+\hat{\mathbf{x}}\rangle + |-\hat{\mathbf{x}}\rangle] \otimes [|+\hat{\mathbf{x}}\rangle + |-\hat{\mathbf{x}}\rangle] \\ &= \frac{1}{2} [|+\hat{\mathbf{x}}, +\hat{\mathbf{x}}\rangle + |+\hat{\mathbf{x}}, -\hat{\mathbf{x}}\rangle + |-\hat{\mathbf{x}}, +\hat{\mathbf{x}}\rangle + |-\hat{\mathbf{x}}, -\hat{\mathbf{x}}\rangle] \end{aligned}$$

The probability of getting both measurements with opposite spins is therefore

$$P(+, -) + P(-, +) = |\langle +\hat{\mathbf{x}}, -\hat{\mathbf{x}}|\alpha\rangle|^2 + |\langle -\hat{\mathbf{x}}, +\hat{\mathbf{x}}|\alpha\rangle|^2 = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$$

(5) First we need to note that

$$|1, +1\rangle_x = |+\hat{\mathbf{x}}, +\hat{\mathbf{x}}\rangle \quad |1, 0\rangle_x = \frac{1}{\sqrt{2}} [|+\hat{\mathbf{x}}, -\hat{\mathbf{x}}\rangle + |-\hat{\mathbf{x}}, +\hat{\mathbf{x}}\rangle] \quad |1, -1\rangle_x = |-\hat{\mathbf{x}}, -\hat{\mathbf{x}}\rangle$$

and then we realize that we already have $|\alpha\rangle = |+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle$ in x -kets from Problem (4). So,

$$\begin{aligned} P(+1) &= |{}_x\langle 1, +1|+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle|^2 = \left| \frac{1}{2} \langle +\hat{\mathbf{x}}, +\hat{\mathbf{x}}|+\hat{\mathbf{x}}, +\hat{\mathbf{x}}\rangle \right|^2 = \frac{1}{4} \\ P(-1) &= |{}_x\langle 1, -1|+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle|^2 = \left| \frac{1}{2} \langle -\hat{\mathbf{x}}, -\hat{\mathbf{x}}|-\hat{\mathbf{x}}, -\hat{\mathbf{x}}\rangle \right|^2 = \frac{1}{4} \\ \text{and } P(0) &= |{}_x\langle 1, 0|+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle|^2 = \left| \frac{1}{\sqrt{2}} [\langle +\hat{\mathbf{x}}, -\hat{\mathbf{x}}|+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle + \langle -\hat{\mathbf{x}}, +\hat{\mathbf{x}}|+\hat{\mathbf{z}}, +\hat{\mathbf{z}}\rangle] \right|^2 \\ &= \left| \frac{1}{2\sqrt{2}} [\langle +\hat{\mathbf{x}}, -\hat{\mathbf{x}}|+\hat{\mathbf{x}}, -\hat{\mathbf{x}}\rangle + \langle -\hat{\mathbf{x}}, +\hat{\mathbf{x}}|-\hat{\mathbf{x}}, +\hat{\mathbf{x}}\rangle] \right|^2 = \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2} \end{aligned}$$

and the three probabilities sum to unity, which they must.

PHYS3701 Intro Quantum Mechanics I HW#9 Due 26 Mar 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

Note: Most or all of these problems are worked out handily in MATHEMATICA.

(1) Show that the Pauli matrix σ_x has the effect of a NOT gate by showing that it gives the expected result on the $|\pm\hat{z}\rangle$ representations of the states $|+\hat{z}\rangle = |0\rangle$ and $|-\hat{z}\rangle = |1\rangle$. Then form the tensor product $\sigma_x \otimes \sigma_x$ and show that it has the expected result on the $|\pm\hat{z}\rangle$ representations of each of the four states $|\pm\hat{z}\rangle \otimes |\pm\hat{z}\rangle$.

(2) A “controlled NOT” gate for two qubits can be constructed as a 4×4 matrix of 2×2 matrices with $\underline{1}$ and $\underline{\sigma}_x$ along the diagonal and zeros otherwise. Show that a CNOT gate flips the second qubit if the first qubit is $|0\rangle$, but does nothing if the first qubit is $|1\rangle$.

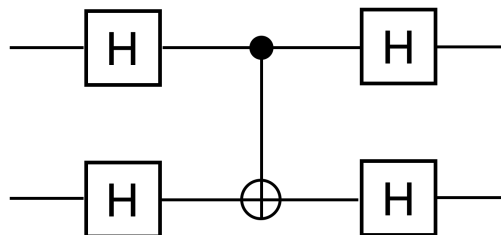
(3) The single qubit Hadamard gate is represented in the $|\pm\hat{z}\rangle$ basis as

$$\underline{H} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

If we interpret $|0\rangle$ and $|1\rangle$ as $|\pm\hat{z}\rangle$ respectively, show how we can use rotations to realize a Hadamard gate. Can you find a solution that does not introduce an overall phase factor?

(4) Show that the two-qubit Hadamard gate $H \otimes H$ acting on the two-qubit state $|0\rangle \otimes |0\rangle$ results in a “fully entangled” state of two qubits. That is, a state which cannot be written simply as a linear combination of one of the qubits times either $|0\rangle$ or $|1\rangle$.

(5) Find the 4×4 matrix representation (in the $|\pm\hat{z}\rangle$ basis) for the following two-qubit gate constructed from four Hadamard gates and a CNOT gate:



Prove that your construction is a unitary transformation.

(1) See the accompanying MATHEMATICA notebook.

(2) See the accompanying MATHEMATICA notebook.

(3) Recall that the rotation operator in the $|\pm\hat{z}\rangle$ basis is

$$\underline{D} = \underline{1} \cos \frac{\phi}{2} - i \underline{\vec{\sigma}} \cdot \hat{\mathbf{n}} \sin \frac{\phi}{2}$$

We can build a Hadamard gate using a 90° rotation about the y -axis, followed by a 180° rotation about the z -axis:

$$\underline{D}_x(\pi) \underline{D}_y\left(\frac{\pi}{2}\right) = \left[-i \underline{\sigma}_x\right] \left[\frac{1}{\sqrt{2}} \underline{1} - \frac{i}{\sqrt{2}} \underline{\sigma}_y\right] = -\frac{i}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} = (-i) \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

where we don't care about the overall phase factor $-i = \exp(-i\pi/2)$. We could also write

$$\begin{bmatrix} \cos(\phi/2) - in_z \sin(\phi/2) & (-n_y - in_x) \sin(\phi/2) \\ (+n_y - in_x) \sin(\phi/2) & \cos(\phi/2) + in_z \sin(\phi/2) \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

and, in principle, use these four equations to solve for n_x , n_y , n_z , and ϕ . However, if we add and subtract the (2,2) and the (1,1) element, we find

$$2 \cos \frac{\phi}{2} = 0 \quad \text{and} \quad -2in_z \sin \frac{\phi}{2} = \frac{2}{\sqrt{2}}$$

so $\phi = \pi$ and $n_z = i/\sqrt{2}$, but n_z needs to be a real number. So there is no way to form a Hadamard gate from a rotation without an overall phase shift.

(4) See the accompanying MATHEMATICA notebook.

(5) See the accompanying MATHEMATICA notebook.

PHYS3701 Intro Quantum Mechanics I HW#10 Due 2 Apr 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

There is only one problem for this week's assignment.

Write a program in MATHEMATICA or some other language to simulate Grover's algorithm. Use as large a number n of qubits as you think you can manage on your classical, digital computer. (It might be more than you would expect.) Remember that this means you will be dealing with column vectors of length $N = 2^n$, and with $N \times N$ matrices.

You should build the $N \times N$ Hadamard matrix using the tensor product of 2×2 matrices, and show that it creates the equal-superposition state from the $|0\rangle$ state. You can build the matrix called " D " by hand instead of constructing it from gates. Remember that the elements are $D_{ij} = -\delta_{ij} + 2/N$. For the oracle, all you need to do is pick a target state, and change the sign of that element.

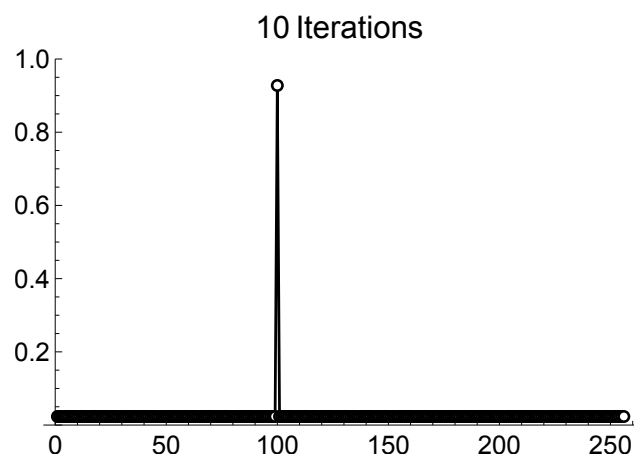
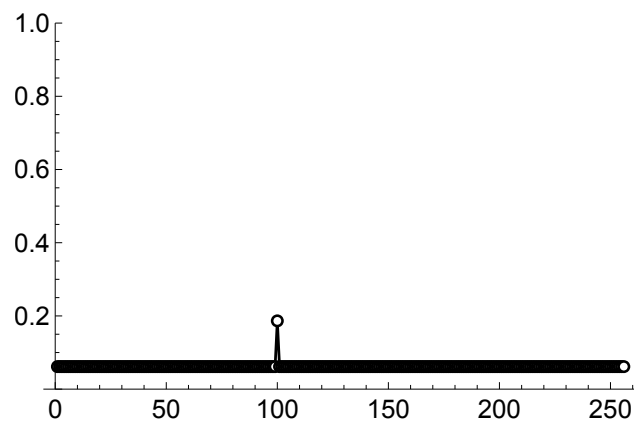
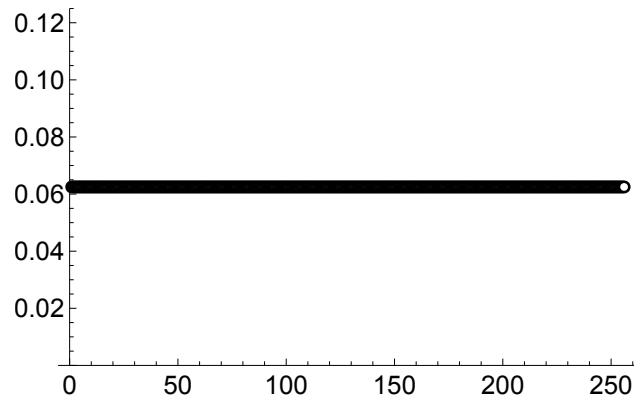
A simple way to check that you've made the equal-superposition state, and to watch the result of each Grover iteration, is to just plot the coefficients of each of the qubits, which is contained in your one N -dimensional qubit. In MATHEMATICA you can do this with ListPlot.

It is tedious to have to put in each Grover iteration by hand. You can try that to start, and watch what happens to the coefficient of your target bit for the first few iterations. But to do a large number of operations, you want to put this in a loop. In MATHEMATICA, I think the simplest way to do this is with For.

What does your array look like for \sqrt{N} iterations? Confirm that this is more or less what you expect. You might find it interesting to also look at what is happening to the other coefficients.

It's only a suggestion, but if you want to make an animation of how the amplitudes change on the qubits with each iteration, that might be a cool demonstration.

See the accompanying MATHEMATICA notebook. Following are the plots of the qubit amplitudes for the initial state, the result of the first iteration, and then ten iterations.



PHYS3701 Intro Quantum Mechanics I HW#11 Due 9 Apr 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) Show that the commutativity of infinitesimal x - and y -translations, in other words $[T(dx \hat{x}), T(dy \hat{y})] = 0$, implies that x - and y -momenta commute, that is $[p_x, p_y] = 0$. You will need to carry out the calculation to second order.

(2) A quantum mechanical “symmetry” can be quantified by some unitary operator \mathcal{S} where, for some observable A , $\langle A \rangle$ is unchanged when the state $|\alpha\rangle \rightarrow \mathcal{S}|\alpha\rangle$.

(a) Show that this symmetry implies that $[\mathcal{S}, A] = 0$.

(b) Assuming $\mathcal{S} = \mathcal{S}(u)$ where u is continuous, use “Weyl’s trick” to write $\mathcal{S}(du)$ in terms of some Hermitian operator \mathcal{G} and show that the symmetry implies that $[\mathcal{G}, A] = 0$.

(c) Illustrate this by showing that the three-dimensional momentum operator \vec{p} is invariant under the translation symmetry operator $T(\vec{a})$. (Don’t be worried if it looks like your illustration is trivial. We will study more about symmetries next semester.)

(3) It is reasonable to define a “vector” as a three component object that transforms under rotations just the way you’d expect. Use this definition and the transformation from Problem (2) above to prove the following relationships for a vector operator $\vec{V} = V_x \hat{x} + V_y \hat{y} + V_z \hat{z}$:

$$[L_z, V_x] = i\hbar V_y \quad [L_z, V_y] = -i\hbar V_x \quad [L_z, V_z] = 0$$

You should notice that this definition implies that angular momentum is indeed a vector.

(4) Recall from our Mathematical Physics course, or in the Concepts textbook Eq (4.8), that the totally antisymmetric symbol ϵ_{ijk} has the property that

$$\epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$$

where the summation over 1, 2, and 3 for repeated indices is implied. Writing the components of the orbital angular momentum operator as

$$L_i = \epsilon_{ijk} r_j p_k \quad \text{where} \quad r_{1,2,3} = x, y, z$$

and using the commutation relations $[r_i, p_j] = i\hbar\delta_{ij}$, show that orbital angular momentum obeys the correct commutation relations for generalized angular momentum that we derived several weeks ago, namely

$$[L_i, L_j] = i\hbar\epsilon_{ijk} L_k$$

(5) Use the techniques from Problem (4), including writing out $[r_i, p_j] = i\hbar\delta_{ij}$ in order to “flip” position and momentum, to prove the relation

$$\vec{L}^2 = \vec{r}^2 \vec{p}^2 - (\vec{r} \cdot \vec{p})^2 + i\hbar \vec{r} \cdot \vec{p}$$

(1) Just write things out to second order and it all falls out. First,

$$\begin{aligned} T(dx \hat{\mathbf{x}}) &= e^{-ip_x dx/\hbar} = 1 + \frac{-ip_x dx}{\hbar} + \frac{1}{2!} \left(\frac{-ip_x dx}{\hbar} \right)^2 + \mathcal{O}(dx^3) \\ &= 1 - \frac{i}{\hbar} p_x dx - \frac{1}{2\hbar^2} p_x^2 dx^2 + \mathcal{O}(dx^3) \\ T(dy \hat{\mathbf{y}}) &= e^{-ip_y dy/\hbar} = 1 - \frac{i}{\hbar} p_y dy - \frac{1}{2\hbar^2} p_y^2 dy^2 + \mathcal{O}(dx^3) \end{aligned}$$

Therefore $T(dx \hat{\mathbf{x}})T(dy \hat{\mathbf{y}}) = T(dy \hat{\mathbf{y}})T(dx \hat{\mathbf{x}})$ means that

$$\begin{aligned} &1 - \frac{i}{\hbar} p_x dx - \frac{1}{2\hbar^2} p_x^2 dx^2 - \frac{i}{\hbar} p_y dy - \frac{1}{\hbar^2} p_x p_y dx dy - \frac{1}{2\hbar^2} p_y^2 dy^2 + \mathcal{O}(dx^3) + \mathcal{O}(dx^2 dy) \\ &= 1 - \frac{i}{\hbar} p_y dy - \frac{1}{2\hbar^2} p_y^2 dy^2 - \frac{i}{\hbar} p_x dx - \frac{1}{\hbar^2} p_y p_x dx dy - \frac{1}{2\hbar^2} p_x^2 dx^2 + \mathcal{O}(dy^3) + \mathcal{O}(dx dy^2) \end{aligned}$$

and most everything on the left and right cancels, leaving us with $p_x p_y = p_y p_x$.

(2) Since $|\alpha\rangle \rightarrow \mathcal{S}|\alpha\rangle$ means that $\langle\alpha| \rightarrow \langle\alpha|\mathcal{S}^\dagger$, the mathematical statement of a symmetry operation is $\langle\alpha|\mathcal{S}^\dagger A \mathcal{S}|\alpha\rangle = \langle\alpha|A|\alpha\rangle$ for an arbitrary state $|\alpha\rangle$. In other words, $\mathcal{S}^\dagger A \mathcal{S} = A$. However, $\mathcal{S}^\dagger \mathcal{S} = 1$ since \mathcal{S} is unitary. So multiply both sides by \mathcal{S} to get $A \mathcal{S} = \mathcal{S} A$ which is the same as writing $[\mathcal{S}, A] = 0$. Now, Weyl's trick is just a way to write a unitary operator with a continuous variable in terms of a Hermitian operator, namely

$$\mathcal{S} = 1 - \frac{i}{\hbar} \mathcal{G} du$$

which insures that \mathcal{S} is unitary for any Hermitian \mathcal{G} . Therefore $\mathcal{S}^\dagger(du)A\mathcal{S}(du) = A$ becomes

$$\left[1 + \frac{i}{\hbar} \mathcal{G} du \right] A \left[1 - \frac{i}{\hbar} \mathcal{G} du \right] = A \quad \text{or} \quad \mathcal{G}A - A\mathcal{G} = [\mathcal{G}, A] = 0$$

keeping terms to first order only. This is trivial to illustrate with the translation operator and momentum. Just write it out to get

$$T^\dagger(\vec{a}) \vec{p} T(\vec{a}) = e^{i\vec{p}\cdot\vec{a}} \vec{p} e^{-i\vec{p}\cdot\vec{a}} = e^{i\vec{p}\cdot\vec{a}} e^{-i\vec{p}\cdot\vec{a}} \vec{p} = \vec{p}$$

since all components of the momentum operator commute with each other.

(3) If you rotate a vector \vec{V} about the z -axis through an angle ϕ , you expect that

$$V_x \rightarrow V_x \cos \phi - V_y \sin \phi \quad V_y \rightarrow V_x \sin \phi + V_y \cos \phi \quad V_z \rightarrow V_z$$

A quantum mechanical rotation about the z -axis is given by the unitary operator

$$e^{-i\epsilon L_z/\hbar} = 1 - \frac{i}{\hbar} \epsilon L_z$$

for an infinitesimal angle $\phi = \epsilon$. Using what we now know about symmetry operations,

$$\begin{aligned} e^{i\epsilon L_z/\hbar} V_x e^{-i\epsilon L_z/\hbar} &= \left[1 + \frac{i}{\hbar} \epsilon L_z \right] V_x \left[1 - \frac{i}{\hbar} \epsilon L_z \right] = V_x + \frac{i}{\hbar} \epsilon [L_z, V_x] + \mathcal{O}(\epsilon^2) \\ &= V_x \cos \epsilon - V_y \sin \epsilon = V_x - \epsilon V_y + \mathcal{O}(\epsilon^2) \end{aligned}$$

Therefore $[L_z, V_x] = i\hbar V_y$. Similarly

$$\begin{aligned} e^{i\epsilon L_z/\hbar} V_y e^{-i\epsilon L_z/\hbar} &= \left[1 + \frac{i}{\hbar}\epsilon L_z\right] V_y \left[1 - \frac{i}{\hbar}\epsilon L_z\right] = V_y + \frac{i}{\hbar}\epsilon [L_z, V_y] + \mathcal{O}(\epsilon^2) \\ &= V_x \sin \epsilon + V_y \cos \epsilon = \epsilon V_x + V_y + \mathcal{O}(\epsilon^2) \end{aligned}$$

Therefore $[L_z, V_y] = -i\hbar V_x$. Finally

$$\begin{aligned} e^{i\epsilon L_z/\hbar} V_z e^{-i\epsilon L_z/\hbar} &= \left[1 + \frac{i}{\hbar}\epsilon L_z\right] V_z \left[1 - \frac{i}{\hbar}\epsilon L_z\right] = V_z + \frac{i}{\hbar}\epsilon [L_z, V_z] + \mathcal{O}(\epsilon^2) \\ &= V_z \end{aligned}$$

and so $[L_z, V_z] = 0$.

(4) This is all pretty straightforward but you have to be careful with indices. First,

$$[L_i, L_j] = [\epsilon_{imn} r_m p_n, \epsilon_{jlk} r_l p_k] = \epsilon_{imn} \epsilon_{jlk} r_m p_n r_l p_k - \epsilon_{imn} \epsilon_{jlk} r_l p_k r_m p_n$$

Now flip the order of the “ pr ” products in the middle so the r 's are on the left and the p 's are on the right in both terms. We have

$$\begin{aligned} \epsilon_{imn} \epsilon_{jlk} r_m p_n r_l p_k &= \epsilon_{imn} \epsilon_{jlk} r_m (r_l p_n - i\hbar \delta_{ln}) p_k = \epsilon_{imn} \epsilon_{jlk} r_m r_l p_n p_k - i\hbar \epsilon_{imn} \epsilon_{jnk} r_m p_k \\ \epsilon_{imn} \epsilon_{jlk} r_l p_k r_m p_n &= \epsilon_{imn} \epsilon_{jlk} r_l (r_m p_k - i\hbar \delta_{qm}) p_n = \epsilon_{imn} \epsilon_{jlk} r_l r_m p_k p_n - i\hbar \epsilon_{imn} \epsilon_{jlm} r_l p_n \end{aligned}$$

Note that the first terms on the right of each of these two equations are equal, because positions commute with positions and momenta commute with momenta. Therefore

$$\begin{aligned} [L_i, L_j] &= i\hbar (-\epsilon_{imn} \epsilon_{jnk} r_m p_k + \epsilon_{imn} \epsilon_{jlm} r_l p_n) = i\hbar (\epsilon_{nim} \epsilon_{njq} r_m p_q - \epsilon_{min} \epsilon_{mj} r_l p_n) \\ &= i\hbar (\delta_{ij} \delta_{mq} r_m p_q - \delta_{iq} \delta_{mj} r_m p_q - \delta_{ij} \delta_{nl} r_l p_n + \delta_{il} \delta_{nj} r_l p_n) \\ &= i\hbar (\delta_{ij} r_m p_m - \delta_{iq} \delta_{mj} r_m p_q - \delta_{ij} r_n p_n + \delta_{il} \delta_{nj} r_l p_n) \\ &= i\hbar (-\delta_{iq} \delta_{mj} r_m p_q + \delta_{il} \delta_{nj} r_l p_n) \\ &= i\hbar (-\delta_{in} \delta_{mj} r_m p_n + \delta_{im} \delta_{nj} r_n p_n) \end{aligned}$$

since $r_m p_m = \vec{r} \cdot \vec{p} = r_n p_n$, and in the last step I changed $q \rightarrow n$ and $l \rightarrow m$, which is fine, since they are just dummy summation indices. Now

$$\epsilon_{ijk} L_k = \epsilon_{ijk} \epsilon_{kmn} r_m p_n = \epsilon_{kij} \epsilon_{kmn} r_m p_n = \delta_{im} \delta_{jn} r_m p_n - \delta_{in} \delta_{jm} r_m p_n$$

which is the same as the last line above. Therefore we have proven that

$$[L_i, L_j] \epsilon_{ijk} L_k$$

(5) For whatever it's worth, this is in fact carried out in MQM3e, Equation (3.226), albeit with a slightly different notation (x for r) and keeping the summation signs (for some reason).

$$\begin{aligned} \vec{L}^2 &= \epsilon_{ijk} r_i p_j \epsilon_{lmk} r_l p_m \\ &= (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) r_i p_j r_l p_m \\ &= [\delta_{il} \delta_{jm} r_i (r_l p_j - i\hbar \delta_{jl}) p_m - \delta_{im} \delta_{jl} r_i p_j (p_m r_l + i\hbar \delta_{lm})] \\ &= \vec{r}^2 \vec{p}^2 - i\hbar \vec{r} \cdot \vec{p} - \delta_{im} \delta_{jl} [r_i p_m (r_l p_j - i\hbar \delta_{jl}) + i\hbar \delta_{lm} r_i p_j] \\ &= \vec{r}^2 \vec{p}^2 - (\vec{r} \cdot \vec{p})^2 + i\hbar \vec{r} \cdot \vec{p} \end{aligned}$$

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PHYS3701 Intro Quantum Mechanics I HW#12 Due 16 Apr 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

I would encourage you to use MATHEMATICA or some other symbolic manipulation problem to work through at least some of these problems.

(1) Show by explicit calculation that the kinetic energy of two masses m_1 and m_2 is

$$\frac{1}{2m_1}\vec{p}_1^2 + \frac{1}{2m_2}\vec{p}_2^2 = \frac{1}{2M}\vec{P}^2 + \frac{1}{2m}\vec{p}^2$$

where $M \equiv m_1 + m_2$, $m = m_1 m_2 / M$, $\vec{P} = \vec{p}_1 + \vec{p}_2$, and $\vec{p} = (m_2 \vec{p}_1 - m_1 \vec{p}_2) / M$.

(2) A three-dimensional spatial wave function over all space has the form

$$\psi(\vec{r}) = N(x + y + 2z)e^{-\alpha^2 r^2}$$

where α is a real constant.

- Find the normalization constant N . (You can assume it is real.)
- Determine the possible results from a measurement of L_z , and the probabilities that they are in fact the result of a measurement.
- Determine the possible results from a measurement of \vec{L}^2 , and the probabilities that they are in fact the result of a measurement.

(3) Defining $L_{\pm} \equiv L_x \pm iL_y$ and the expression we derived for $\langle \vec{r}' | \vec{L} | \alpha \rangle$, show that

$$\langle \vec{r}' | L_{\pm} | \alpha \rangle = -i\hbar e^{\pm i\phi} \left(\pm i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \langle \vec{r}' | \alpha \rangle$$

(4) Use the result of Problem (3) to show that

$$\langle \vec{r}' | \vec{L}^2 | \alpha \rangle = -\hbar^2 \left[\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \right] \langle \vec{r}' | \alpha \rangle$$

(5) A certain spherical harmonic is given by

$$Y_{\ell}^m(\theta, \phi) = \frac{3}{8} \sqrt{\frac{5}{2\pi}} e^{-2i\phi} \sin^2 \theta (7 \cos^2 \theta - 1)$$

- Show that this function is properly normalized.
- Determine the values of ℓ and m . You might want to use the result of Problem (4), along with the analogous result for the operator L_z .

(1) We could just substitute into the right and show that it equals the left, but maybe there's something to be learned by going in the other direction. So,

$$\begin{aligned}
 \vec{p}_1 + \vec{p}_2 &= \vec{P} \\
 \text{and } m_2\vec{p}_1 - m_1\vec{p}_2 &= M\vec{p} \\
 \text{so } (m_1 + m_2)\vec{p}_1 &= M\vec{p}_1 = m_1\vec{P} + M\vec{p} \\
 \text{therefore } \vec{p}_1 &= \vec{p} + \frac{m_1}{M}\vec{P} \\
 \text{plus } (m_1 + m_2)\vec{p}_2 &= M\vec{p}_2 = m_2\vec{P} - M\vec{p} \\
 \text{and, finally } \vec{p}_2 &= -\vec{p} + \frac{m_2}{M}\vec{P}
 \end{aligned}$$

Now just proceed with the algebra.

$$\begin{aligned}
 \frac{1}{2m_1}\vec{p}_1^2 + \frac{1}{2m_2}\vec{p}_2^2 &= \frac{1}{2m_1}\left(\vec{p} + \frac{m_1}{M}\vec{P}\right)^2 + \frac{1}{2m_2}\left(-\vec{p} + \frac{m_2}{M}\vec{P}\right)^2 \\
 &= \frac{1}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\vec{p}^2 + \frac{1}{M}\vec{p}\cdot\vec{P} - \frac{1}{M}\vec{p}\cdot\vec{P} + \frac{1}{2}\left(\frac{m_1}{M^2} + \frac{m_2}{M^2}\right)\vec{P}^2 \\
 &= \frac{1}{2m}\vec{p}^2 + \frac{1}{2M}\vec{P}^2
 \end{aligned}$$

(2) See the accompanying MATHEMATICA notebook. The total angular momentum quantum number is $\ell = 1$ so the only possible result of a measurement of \vec{L}^2 is $2\hbar^2$. The probabilities to measure $m = 0, \pm 1$ are $2/3$ and $1/6$, respectively.

(3) Start with the expression we derived in class for $\langle \vec{r}' | \vec{L} | \alpha \rangle$ in spherical coordinates and then convert the unit vectors to the Cartesian form using Concepts Equations (4.15).

$$\begin{aligned}
 \langle \vec{r}' | \vec{L} | \alpha \rangle &= \frac{\hbar}{i} \left[\hat{\phi} \frac{\partial}{\partial \theta} - \hat{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right] \langle \vec{r}' | \alpha \rangle \\
 &= \frac{\hbar}{i} \left[(-\hat{x} \sin \phi + \hat{y} \cos \phi) \frac{\partial}{\partial \theta} - (\hat{x} \cos \phi \cos \theta + \hat{y} \sin \phi \cos \theta - \hat{z} \sin \theta) \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right] \langle \vec{r}' | \alpha \rangle \\
 &= \frac{\hbar}{i} \left[\hat{x} \left(-\sin \phi \frac{\partial}{\partial \theta} - \cos \phi \cot \theta \frac{\partial}{\partial \phi} \right) + \hat{y} \left(\cos \phi \frac{\partial}{\partial \theta} - \sin \phi \cot \theta \frac{\partial}{\partial \phi} \right) + \hat{z} \frac{\partial}{\partial \phi} \right] \langle \vec{r}' | \alpha \rangle
 \end{aligned}$$

Therefore

$$\langle \vec{r}' | L_x | \alpha \rangle = \frac{\hbar}{i} \left(-\sin \phi \frac{\partial}{\partial \theta} - \cos \phi \cot \theta \frac{\partial}{\partial \phi} \right) \langle \vec{r}' | \alpha \rangle$$

and

$$\langle \vec{r}' | L_y | \alpha \rangle = \frac{\hbar}{i} \left(\cos \phi \frac{\partial}{\partial \theta} - \sin \phi \cot \theta \frac{\partial}{\partial \phi} \right) \langle \vec{r}' | \alpha \rangle$$

Hence

$$\begin{aligned}
\langle \vec{r}' | L_{\pm} | \alpha \rangle &= \langle \vec{r}' | (L_x \pm iL_y) | \alpha \rangle \\
&= \frac{\hbar}{i} \left[(-\sin \phi \pm i \cos \phi) \frac{\partial}{\partial \theta} - (\cos \phi \pm i \sin \phi) \cot \theta \frac{\partial}{\partial \phi} \right] \langle \vec{r}' | \alpha \rangle \\
&= -i\hbar \left[\pm i (\cos \phi \pm i \sin \phi) \frac{\partial}{\partial \theta} - (\cos \phi \pm i \sin \phi) \cot \theta \frac{\partial}{\partial \phi} \right] \langle \vec{r}' | \alpha \rangle \\
&= -i\hbar e^{\pm i\phi} \left[\pm i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right] \langle \vec{r}' | \alpha \rangle
\end{aligned}$$

which is what we set out to prove.

(4) We know from our study of the general properties of angular momentum that

$$\vec{J}^2 = J_x^2 + J_y^2 + J_z^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2$$

so interpret \vec{J} as \vec{L} and proceed with the derivatives. Using the dreaded “arrow” notation for the sake of brevity, we first write

$$L_z^2 \rightarrow \left(\frac{\hbar}{i} \frac{\partial}{\partial \phi} \right) \left(\frac{\hbar}{i} \frac{\partial}{\partial \phi} \right) = -\hbar^2 \frac{\partial^2}{\partial \phi^2}$$

Remembering that

$$\frac{d}{d\theta} \cot \theta = \frac{d \cos \theta}{d\theta \sin \theta} = \frac{-\sin^2 \theta - \cos^2 \theta}{\sin^2 \theta} = -\frac{1}{\sin^2 \theta}$$

we can then do the derivative forms of L_+ and L_- to get

$$\begin{aligned}
L_+L_- &\rightarrow \left(-i\hbar e^{i\phi} \left[i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right] \right) \left(-i\hbar e^{-i\phi} \left[-i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right] \right) \\
&= -\hbar^2 e^{i\phi} \left(e^{-i\phi} \frac{\partial^2}{\partial \theta^2} + ie^{-i\phi} \frac{1}{\sin^2 \theta} \frac{\partial}{\partial \phi} - ie^{-i\phi} \cot \theta \frac{\partial^2}{\partial \theta \partial \phi} \right. \\
&\quad \left. + ie^{-i\phi} \cot \theta \left[-i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right] + ie^{-i\phi} \cot \theta \frac{\partial}{\partial \theta} + e^{-i\phi} \cot^2 \theta \frac{\partial^2}{\partial \phi^2} \right) \\
L_-L_+ &\rightarrow \left(-i\hbar e^{-i\phi} \left[-i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right] \right) \left(-i\hbar e^{i\phi} \left[i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right] \right) \\
&= -\hbar^2 e^{-i\phi} \left(e^{i\phi} \frac{\partial^2}{\partial \theta^2} - ie^{i\phi} \frac{1}{\sin^2 \theta} \frac{\partial}{\partial \phi} + ie^{i\phi} \cot \theta \frac{\partial^2}{\partial \theta \partial \phi} \right. \\
&\quad \left. - ie^{i\phi} \cot \theta \left[i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right] - ie^{i\phi} \cot \theta \frac{\partial}{\partial \theta} - e^{i\phi} \cot^2 \theta \frac{\partial^2}{\partial \phi^2} \right)
\end{aligned}$$

Lots of things cancel when we add these, including $e^{i\phi}e^{-i\phi} = 1$, so

$$L_+L_- + L_-L_+ \rightarrow -2\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \cot^2 \theta \frac{\partial^2}{\partial \phi^2} \right)$$

Combining this with L_z^2 we get

$$\vec{L}^2 \rightarrow -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \cot^2 \theta \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial \phi^2} \right)$$

Finally, we realize that

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) = \frac{\partial^2}{\partial \theta^2} + \frac{1}{\sin \theta} \cos \theta \frac{\partial}{\partial \theta} = \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta}$$

and

$$\cot^2 \theta + 1 = \frac{\cos^2 \theta}{\sin^2 \theta} + 1 = \frac{\cos^2 \theta + \sin^2 \theta}{\sin^2 \theta} = \frac{1}{\sin^2 \theta}$$

so we indeed end up with what we were trying to prove.

(5) See the accompanying MATHEMATICA notebook. This is $Y_2^{-2}(\theta, \phi)$.

PHYS3701 Intro Quantum Mechanics I HW#13 Due 23 Apr 2024

This homework assignment is due at the start of class on the date shown. Please submit a PDF of your solutions to the Canvas page for the course.

(1) We showed in class that when $r \rightarrow 0$, the radial wave function for central potential problems can, in principle, have the form

$$R(r) = Ar^l + \frac{B}{r^{l+1}}$$

where A and B are constants. By integrating the probability flux $\vec{j} = (\hbar/m)\text{Im}(\psi^*\vec{\nabla}\psi)$ over a small sphere around the origin, show that this would imply that the origin is a source of probability of both A and B are nonzero have a nonzero relative complex phase.

(2) Find the energy eigenvalues, and plot the radial eigenfunctions, for the following cases of an infinite spherical box of radius a :

- (a) The lowest energy level (aka the ground state) with $l = 0$
- (b) The first excited state with $l = 0$
- (c) The second excited state with $l = 2$

(3) Find the lowest energy eigenvalues with $l = 0$ for a finite spherical box with radius a finite walls of height $V_0 = \hbar^2\beta^2/2ma^2$, where $\beta = 4, 10, 25$, and 100 . (You need to do this numerically with MATHEMATICA or some other application.) Show that these results approach what you found in Problem (2) above.

(4) Construct all of the wave functions $\psi_{nlm}(r, \theta, \phi)$ for the eigenstates corresponding to the first excited state energy eigenvalue of the isotropic three dimensional harmonic oscillator for a particle of mass m and natural frequency ω . Using MATHEMATICA or some other graphing application, make a three dimensional plot of the probability density $\psi_{nlm}^*(r, \theta, \phi)\psi_{nlm}(r, \theta, \phi)$ for each of the wave functions.

(5) Look up the phenomenon called “magic numbers” in nuclear physics. Imagine that protons and neutrons move independently in an isotropic harmonic oscillator potential, and compare what you’d predict for the first five magic numbers to what is observed. Don’t forget about the Paul Exclusion Principle, which I suppose you learned at some time.

(1) We are going to calculate the surface integral over a sphere centered at the origin, so all we need is the radial component of the flux and we can ignore the spherical harmonics in the wave function. (They will just integrate to unity over the sphere.) Therefore we have

$$j_r(r) = \frac{\hbar}{m} \text{Im} \left[\left(A^* r^l + \frac{B^*}{r^{l+1}} \right) \left(l A r^{l-1} - (l+1) \frac{B}{r^{l+2}} \right) \right] = \frac{\hbar}{m} \text{Im} \left[\frac{l B^* A}{r^2} - \frac{(l+1) A^* B}{r^2} \right]$$

If we write $B = c A e^{i\delta}$ where c , A , and δ are real, then $B^* A = c A^2 e^{-i\delta}$ and $A^* B = c A^2 e^{i\delta}$, so the radial flux is

$$j_r(r) = \frac{\hbar}{m} c A^2 \frac{1}{r^2} \text{Im} [l e^{-i\delta} - (l+1) e^{i\delta}] = -\frac{\hbar}{m} c A^2 \frac{1}{r^2} (2l+1) \sin \delta$$

The factor of $1/r^2$ is critical, because integrating over a (tiny) sphere of radius R means multiplying by $4\pi R^2$ and so the flux out of the origin is

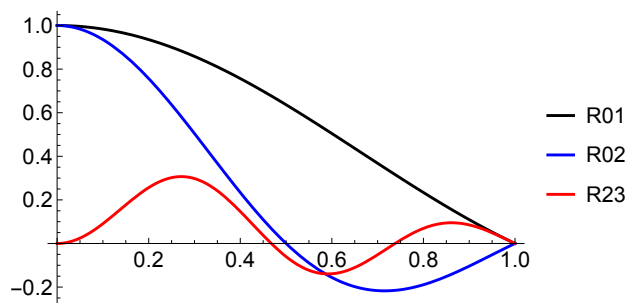
$$\oint \vec{j} \cdot d\vec{S} = -\frac{4\pi\hbar}{m} c A^2 (2l+1) \sin \delta$$

which is nonzero as $r \rightarrow 0$ if the relative phase δ is nonzero.

(2) See the accompanying MATHEMATICA notebook. The energy eigenvalues are

$$\begin{aligned} E_{l=0,1} &= \frac{\hbar^2}{2ma^2} (\pi^2) = \frac{\hbar^2}{2ma^2} 9.87 \\ E_{l=0,2} &= \frac{\hbar^2}{2ma^2} (2\pi)^2 = \frac{\hbar^2}{2ma^2} 39.5 \\ E_{l=2,3} &= \frac{\hbar^2}{2ma^2} (12.32)^2 = \frac{\hbar^2}{2ma^2} 152 \end{aligned}$$

and the (unnormalized) wave functions are



(3) Parameterize the energy eigenvalue as $E = \hbar^2 \alpha^2 / 2ma^2$. The radial wave function for $r \leq a$ is $A j_0(kr) = A \sin(\alpha r/a) / (\alpha r/a)$. For $r \geq a$, the wave function satisfies

$$R(r) = \frac{u(r)}{r} \quad \text{where} \quad -\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \frac{\hbar^2 \beta^2}{2ma^2} u(r) = \frac{\hbar^2 \alpha^2}{2ma^2} u(r)$$

For bound states, we need $\alpha^2 < \beta^2$ so $\gamma^2 \equiv \beta^2 - \alpha^2 > 0$. Therefore $u''(r) = (\gamma/a)^2 u(r)$ and

$$u(r) \propto \exp\left(-\frac{\gamma r}{a}\right) \quad \text{and} \quad R(r) = B \frac{a}{r} \exp\left(-\frac{\gamma r}{a}\right) \quad \text{for} \quad r \geq a$$

The procedure is now familiar from 1D wave mechanics. We require $j_0(ka) = R(a)$ and $j'_0(ka) = R'(a)$ and then impose that the determinant is zero in the matrix equation for A and B . At this point, see the accompanying MATHEMATICA notebook. We find the determinant equation to be

$$\frac{\sqrt{\beta^2 - \alpha^2} \sin(\alpha)}{\alpha} + \cos(\alpha) = 0$$

and then find the zeros of this to get $\alpha = 2.47, 2.85, 3.02, 3.11$ for $\beta = 4, 10, 25, 100$, respectively. As expected, the values for α approach π as the well gets very deep.

(4) If we approach this using Cartesian coordinates, then the energy eigenvalues are

$$E_n = \left(N + \frac{3}{2}\right) \quad \text{where} \quad N = n_x + n_y + n_z = 0, 1, 2, \dots$$

so the first excited corresponds to one of n_x, n_y , or n_z equal to unity and the other two equal to zero. The eigenfunctions are just the products of the first excited and ground states of the simple harmonic oscillator in one dimension. Writing the wave function as ψ_{n_x, n_y, n_z} ,

$$\begin{aligned} \psi_{1,0,0} &= \left[\frac{4}{\pi} \left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} x e^{-m\omega x^2/2\hbar} \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega y^2/2\hbar} e^{-m\omega z^2/2\hbar} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \left[\frac{4}{\pi} \left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} x e^{-m\omega r^2/2\hbar} \\ \psi_{0,1,0} &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \left[\frac{4}{\pi} \left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} y e^{-m\omega r^2/2\hbar} \\ \psi_{0,0,1} &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \left[\frac{4}{\pi} \left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} z e^{-m\omega r^2/2\hbar} \end{aligned}$$

Now we need to find the linear combinations of these that are angular momentum eigenstates, We know how to write x, y , and z in terms of spherical harmonics using

$$Y_1^1(\theta, \phi) = -\frac{1}{2} \sqrt{\frac{3}{2\pi}} \frac{x + iy}{r} \quad Y_1^{-1}(\theta, \phi) = +\frac{1}{2} \sqrt{\frac{3}{2\pi}} \frac{x - iy}{r} \quad Y_1^0(\theta, \phi) = \frac{1}{2} \sqrt{\frac{3}{\pi}} \frac{z}{r}$$

so the appropriate normalized linear combinations are

$$\begin{aligned} \frac{1}{\sqrt{2}} [\psi_{1,0,0} + i\psi_{0,1,0}] &= -\frac{1}{\sqrt{2}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \left[\frac{4}{\pi} \left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} \left[2\sqrt{\frac{2\pi}{3}} r Y_1^1(\theta, \phi)\right] e^{-m\omega r^2/2\hbar} \\ \frac{1}{\sqrt{2}} [\psi_{1,0,0} - i\psi_{0,1,0}] &= +\frac{1}{\sqrt{2}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \left[\frac{4}{\pi} \left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} \left[2\sqrt{\frac{2\pi}{3}} r Y_1^{-1}(\theta, \phi)\right] e^{-m\omega r^2/2\hbar} \\ \text{and} \quad \psi_{0,0,1} &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \left[\frac{4}{\pi} \left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} \left[2\sqrt{\frac{\pi}{3}} r Y_1^0(\theta, \phi)\right] e^{-m\omega r^2/2\hbar} \end{aligned}$$

Writing these with a common overall normalization constant N and the dimensionless length $\rho = r(m\omega/\hbar)^{1/2}$, we get the eigenfunctions $\psi_{1,l,m}$ (where the 1 means first excited state),

$$\begin{aligned} \psi_{1,1,1}(r, \theta, \phi) &= N Y_1^1(\theta, \phi) \rho e^{-\rho^2/2} \\ \psi_{1,1,-1}(r, \theta, \phi) &= N Y_1^{-1}(\theta, \phi) \rho e^{-\rho^2/2} \\ \text{and} \quad \psi_{1,1,0}(r, \theta, \phi) &= N Y_1^0(\theta, \phi) \rho e^{-\rho^2/2} \end{aligned}$$

which would seem to be correct. Of course, we could have gotten here by solving the problem in spherical coordinates as a central force problem. In this case, as discussed in class, the energy levels are

$$E_n = \left(N + \frac{3}{2} \right) = \left(2q + l + \frac{3}{2} \right) \quad \text{where} \quad q = 0, 1, 2, \dots$$

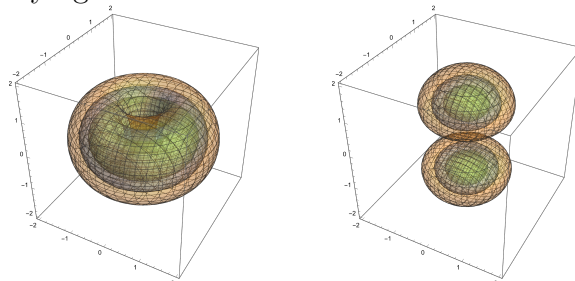
where the radial eigenfunctions $R(r) = u(\rho)/\rho$ and

$$u(\rho) = \rho^{l+1} e^{-\rho^2/2} f(\rho) \quad \text{where} \quad f(\rho) = \sum_{n=0}^{\infty} a_n \rho^n$$

with the a_n is nonzero only for even n , and are determined by the recursion relation

$$a_{n+2} = \frac{2n + 2l + 3 - \lambda}{(n + 2)(n + 2l + 3)} a_n \quad \text{where} \quad \lambda = \frac{2E_n}{\hbar\lambda}$$

and the series must terminate at $n = 2q$. In this problem, the first excited states are for $q = 0$ and $l = 1$, and the radial wave function is proportional to $u(\rho)/\rho = \rho e^{-\rho^2/2}$, which agrees with what we found using Cartesian coordinates. The plots of the probability densities are below, from the accompanying MATHEMATICA notebook.



where the plot on the left is for the $m = 0$ state, and the right is for the $m = \pm 1$ states (which have the same probability density.)

(5) The “magic numbers” of protons or neutrons (aka nucleons) give nuclei that are especially stable against decay because these numbers close the “shells”, similar to closed shells of electrons in atoms. If the nucleons move in a harmonic oscillator potential, this would correspond to filled energy levels for each N . Remembering the Pauli Exclusion Principle, we multiply the degeneracy of each level by two, and add them up to get the magic numbers.

N	l	$\sum_l (2l + 1)$	Sum	$\times 2$	Expt
0	0	1	1	2	2
1	1	3	4	8	8
2	0,2	1 + 5 = 6	10	20	20
3	1,3	3 + 7 = 10	20	40	28
4	0,2,4	1 + 5 + 9 = 15	35	70	50

This incredibly simple model of a nucleus works pretty well for the first three shells. After that, the spin-orbit interaction takes over, but realizing that was worth the Nobel Prize to Mayer and Jensen.