Sample Questions II

1) a) What is $\left[\hat{\phi}, \hat{L}_z\right]$?
b) Calculate the root-mean-square deviation $(\Delta\phi)$ for a particle in the uniform state form $-\pi$ to π.

Solution:
a) The position operator $\hat{\phi}$ represents the angle, and $\hat{L}_z$ is the angular momentum operator:

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}.$$

Using this expression, the commutator between $\hat{\phi}$ and $\hat{L}_z$ is calculated as:

$$[\hat{\phi}, \hat{L}_z] = \hat{\phi}\hat{L}_z - \hat{L}_z\hat{\phi}.$$

Substituting $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$ into this:

$$[\hat{\phi}, \hat{L}_z] = \hat{\phi}\left(-i\hbar\frac{\partial}{\partial\phi}\right) - \left(-i\hbar\frac{\partial}{\partial\phi}\right)\hat{\phi}.$$

This simplifies to:

$$[\hat{\phi}, \hat{L}_z] = -i\hbar\left(\hat{\phi}\frac{\partial}{\partial\phi} - \frac{\partial}{\partial\phi}\hat{\phi}\right).$$

Now, let us act on a test function $f(\phi)$ to compute each term in the commutator.

First term: $\hat{\phi}\frac{\partial}{\partial\phi}f(\phi)$

$$\hat{\phi}\frac{\partial}{\partial\phi}f(\phi) = \phi\frac{\partial}{\partial\phi}f(\phi).$$

Second term: $\frac{\partial}{\partial\phi}\hat{\phi}f(\phi)$

$$\frac{\partial}{\partial\phi}\hat{\phi}f(\phi) = \frac{\partial}{\partial\phi}\left(\phi f(\phi)\right).$$

Using the product rule of differentiation:

$$\frac{\partial}{\partial\phi}\left(\phi f(\phi)\right) = f(\phi) + \phi\frac{\partial}{\partial\phi}f(\phi).$$

Now substitute these results into the commutator:

$$[\hat{\phi}, \hat{L}_z]f(\phi) = -i\hbar\left(\phi\frac{\partial}{\partial\phi}f(\phi) - \left(f(\phi) + \phi\frac{\partial}{\partial\phi}f(\phi)\right)\right).$$

$$[\hat{\phi}, \hat{L}_z]f(\phi) = i\hbar f(\phi).$$

b) In this part, we need to calculate the uncertainty in the angle ϕ, denoted as $\Delta\phi$, for a particle in the uniform state $\psi(\phi) = \frac{1}{\sqrt{2\pi}}$, which represents a constant probability density over the interval $[-\pi, \pi]$.

The standard deviation $\Delta\phi$ is given by:

$$\Delta\phi = \sqrt{\langle\hat{\phi}^2\rangle - \langle\hat{\phi}\rangle^2}.$$

The expectation value $\langle\hat{\phi}\rangle$ is given by:

$$\langle\hat{\phi}\rangle = \int_{-\pi}^{\pi} \psi^*(\phi)\, \hat{\phi}\, \psi(\phi)\, d\phi.$$

Since $\psi(\phi) = \frac{1}{\sqrt{2\pi}}$, we have:

$$\langle\hat{\phi}\rangle = \int_{-\pi}^{\pi} \frac{1}{2\pi} \phi\, d\phi = 0.$$

The expectation value of $\hat{\phi}^2$ is:

$$\langle\hat{\phi}^2\rangle = \int_{-\pi}^{\pi} \frac{1}{2\pi} \phi^2\, d\phi.$$

We can evaluate this integral as follows:

$$\langle\hat{\phi}^2\rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} \phi^2\, d\phi = \frac{1}{2\pi} \cdot 2 \int_{0}^{\pi} \phi^2\, d\phi = \frac{1}{\pi} \left[\frac{\phi^3}{3}\right]_0^{\pi} = \frac{\pi^2}{3}.$$

Now, we can compute the uncertainty:

$$\Delta\phi = \sqrt{\langle\hat{\phi}^2\rangle - \langle\hat{\phi}\rangle^2} = \sqrt{\frac{\pi^2}{3} - 0} = \frac{\pi}{\sqrt{3}}.$$

Thus, the root-mean-square deviation $\Delta\phi$ is:

$$\Delta\phi = \frac{\pi}{\sqrt{3}}.$$

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2) Show that $\hat{L}^2$ may be written as:

$$\hat{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right).$$

Solution: To show that $\hat{L}^2$ can be expressed in the given form, we start with its definition and derive the spherical coordinate representation.

The squared angular momentum operator $\hat{L}^2$ is defined as:

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2.$$

The components of the angular momentum operator in Cartesian coordinates are:

$$\hat{L}_x = -i\hbar \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right),$$

$$\hat{L}_y = -i\hbar \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right),$$

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

Transforming to Spherical Coordinates

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta.$$

The differential operators in spherical coordinates are:

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi},$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi},$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}.$$

It can be shown that $\hat{L}^2$ in spherical coordinates takes the form:

$$\hat{L}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

Now, we simplify the term $\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)$:

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

Substituting this back into the expression for $\hat{L}^2$, we have:

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

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3) Prove that:

$$\hat{L}^2 Y_2^2 = 6\hbar^2 Y_2^2$$
$$\hat{L}_z Y_2^2 = 2\hbar Y_2^2$$

The function Y_2^2: $\left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{2i\phi}$.

Solution:

The operator $\hat{L}_z$ is defined as:

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}.$$

Applying $\hat{L}_z$ to Y_2^2:

$$\hat{L}_z Y_2^2 = -i\hbar\frac{\partial}{\partial\phi}\left[\left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{2i\phi}\right].$$

Since $\sin^2\theta$ is independent of ϕ, we have:

$$\frac{\partial}{\partial\phi}e^{2i\phi} = 2ie^{2i\phi}.$$

$$\hat{L}_z Y_2^2 = -i\hbar \cdot 2i \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{2i\phi}.$$

Simplifying:

$$\hat{L}_z Y_2^2 = 2\hbar \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{2i\phi} = 2\hbar Y_2^2.$$

The operator $\hat{L}^2$ in spherical coordinates is given by:

$$\hat{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

<u>Applying $\hat{L}^2$ to Y_2^2:</u>

$$Y_2^2 = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{2i\phi}.$$

Second derivative with respect to ϕ:

$$\frac{\partial^2}{\partial\phi^2} e^{2i\phi} = 4i^2 e^{2i\phi} = -4e^{2i\phi}.$$

So:

$$\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} Y_2^2 = -\frac{4}{\sin^2\theta}\left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{2i\phi} = -4\left(\frac{15}{32\pi}\right)^{1/2} e^{2i\phi}.$$

Derivatives with respect to θ:

$$\frac{\partial}{\partial\theta}(\sin^2\theta) = 2\sin\theta\cos\theta,$$

$$\frac{\partial^2}{\partial\theta^2}(\sin^2\theta) = 2(\cos^2\theta - \sin^2\theta).$$

Substitute back into $\hat{L}^2 Y_2^2$:

$$\hat{L}^2 Y_2^2 = 6\hbar^2 Y_2^2.$$

Alternate: The function Y_2^2 is given by:

$$Y_2^2 = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{2i\phi},$$

which corresponds to the state $|l = 2, m = 2\rangle$. Therefore, we can write:

$$|2, 2\rangle = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{2i\phi}.$$

Action of $\hat{L}^2$:

$$\hat{L}^2 |l, m\rangle = l(l+1)\hbar^2 |l, m\rangle.$$

For $l = 2$:

$$\hat{L}^2 |2, 2\rangle = 2(2+1)\hbar^2 |2, 2\rangle = 6\hbar^2 |2, 2\rangle.$$

Action of $\hat{L}_z$:

$$\hat{L}_z|l,m\rangle = m\hbar|l,m\rangle.$$

For $m = 2$:

$$\hat{L}_z|2,2\rangle = 2\hbar|2,2\rangle.$$

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4) At a given instant of time, a rigid rotator is in the state:

$$\varphi(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\sin\phi\sin\theta.$$

(a) What possible values of L_z will measurement find, and with what probability will these values occur?
(b) What is $\left\langle \hat{L}_x \right\rangle$ for this state?
(c) What is $\left\langle \hat{L}^2 \right\rangle$ for this state?

Solution:
a) Measurement of L_z:

The operator $\hat{L}_z$ has eigenfunctions $Y_l^m(\theta,\phi)$ in the basis of spherical harmonics:

$$\hat{L}_z Y_l^m(\theta,\phi) = m\hbar Y_l^m(\theta,\phi).$$

To find the possible values of L_z and their probabilities, we need to expand $\varphi(\theta,\phi)$ in terms of the spherical harmonics $Y_l^m(\theta,\phi)$:

$$\varphi(\theta,\phi) = \sum_{l,m} c_{l,m} Y_l^m(\theta,\phi),$$

Given $\varphi(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\sin\phi\sin\theta$, we can express $\sin\phi$ in terms of spherical harmonics:

$$\sin\phi = \frac{e^{i\phi} - e^{-i\phi}}{2i}.$$

The function $\sin\phi\sin\theta$ can be expanded as:

$$\sin\phi\sin\theta = \frac{1}{2i}\sin\theta(e^{i\phi} - e^{-i\phi}).$$

Using the known spherical harmonics:

$$Y_1^{\pm 1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi},$$

we can write:

$$\varphi(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\sin\phi\sin\theta = -\frac{i}{\sqrt{2}}Y_1^1(\theta,\phi) + \frac{i}{\sqrt{2}}Y_1^{-1}(\theta,\phi).$$

Coefficients $c_{1,\pm 1}$:

$$c_{1,1} = -\frac{i}{\sqrt{2}}, \quad c_{1,-1} = \frac{i}{\sqrt{2}}.$$

Possible values of L_z:

- $m = 1$: $L_z = \hbar$ with probability $|c_{1,1}|^2 = \frac{1}{2}$.
- $m = -1$: $L_z = -\hbar$ with probability $|c_{1,-1}|^2 = \frac{1}{2}$.

The possible values of L_z are $\hbar$ and $-\hbar$, each occurring with a probability of $\frac{1}{2}$.
b) Expectation Value $\langle \hat{L}_x \rangle$:

The operator $\hat{L}_x$ can be expressed in terms of $\hat{L}_+$ and $\hat{L}_-$:

$$\hat{L}_x = \frac{\hat{L}_+ + \hat{L}_-}{2},$$

where:

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y.$$

The matrix elements $\langle Y_{l'}^{m'} | \hat{L}_x | Y_l^m \rangle$ are non-zero only when $m' = m \pm 1$. In this case:

$$\langle \hat{L}_x \rangle = \int_0^{2\pi} \int_0^{\pi} \varphi^*(\theta, \phi) \hat{L}_x \varphi(\theta, \phi) \sin\theta \, d\theta \, d\phi.$$

Since $\varphi(\theta, \phi)$ is a linear combination of Y_1^1 and Y_1^{-1}, we need to evaluate:

$$\langle \hat{L}_x \rangle = \frac{1}{2} \left[\langle 1, 1 | \hat{L}_+ | 1, -1 \rangle + \langle 1, -1 | \hat{L}_- | 1, 1 \rangle \right].$$

Calculating these matrix elements, we find:

$$\langle \hat{L}_x \rangle = 0.$$

c) Expectation Value $\langle \hat{L}^2 \rangle$
For $\varphi(\theta, \phi)$, we can use the fact that:

$$\langle \hat{L}^2 \rangle = \sum_{l,m} |c_{l,m}|^2 l(l+1)\hbar^2.$$

Since the state is a combination of Y_1^1 and Y_1^{-1}, both corresponding to $l = 1$:

$$\langle \hat{L}^2 \rangle = 1(1+1)\hbar^2 = 2\hbar^2.$$

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5) Assume that a particle has an orbital angular momentum with z component $\hbar m$ and a square magnitude $\hbar^2 l(l+1)$. Show the following:

a) Show that $\langle L_x \rangle = \langle L_y \rangle = 0$
b) Show that

$$\langle L_x^2 \rangle = \langle L_y^2 \rangle = \frac{\hbar^2 l(l+1) - m^2\hbar^2}{2}$$

Solution:

a) The raising and lowering operators are defined as:

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y, \quad \hat{L}_- = \hat{L}_x - i\hat{L}_y.$$

Action on Eigenstates: For an eigenstate $|l, m\rangle$ of $\hat{L}^2$ and $\hat{L}_z$:

$$\hat{L}_+|l, m\rangle = \hbar\sqrt{l(l+1) - m(m+1)}|l, m+1\rangle,$$

$$\hat{L}_-|l, m\rangle = \hbar\sqrt{l(l+1) - m(m-1)}|l, m-1\rangle.$$

The expectation values $\langle L_x\rangle$ and $\langle L_y\rangle$ in the state $|l, m\rangle$using the operators $\hat{L}_+$ and $\hat{L}_-$:

$$\langle L_x\rangle = \frac{1}{2}\langle l, m|\hat{L}_+ + \hat{L}_-|l, m\rangle$$

$$\langle L_y\rangle = \frac{1}{2i}\langle l, m|\hat{L}_+ - \hat{L}_-|l, m\rangle.$$

The expectation value of $\hat{L}_x$ in the state $|l, m\rangle$ is:

$$\langle L_x\rangle = \langle l, m|\hat{L}_x|l, m\rangle = \frac{1}{2}\left(\langle l, m|\hat{L}_+|l, m\rangle + \langle l, m|\hat{L}_-|l, m\rangle\right).$$

Taking the inner product for the first term:

$$\langle l, m|\hat{L}_+|l, m\rangle = \hbar\sqrt{(l-m)(l+m+1)}\,\langle l, m|l, m+1\rangle\,.$$

Since $|l, m\rangle$ and $|l, m+1\rangle$ are orthogonal for different m, we have:

$$\langle l, m|l, m+1\rangle = 0.$$

Similarly, for the second term:

$$\langle l, m|\hat{L}_-|l, m\rangle = \hbar\sqrt{(l+m)(l-m+1)}\,\langle l, m|l, m-1\rangle\,.$$

Again, due to orthogonality:

$$\langle l, m|l, m-1\rangle = 0,$$

Substituting these results back into the expectation value of $\hat{L}_x$:

$$\langle L_x\rangle = \frac{1}{2}\left(\langle l, m|\hat{L}_+|l, m\rangle + \langle l, m|\hat{L}_-|l, m\rangle\right) = \frac{1}{2}(0+0) = 0.$$

Similarly, the expectation value of $\hat{L}_y$ is:

$$\langle L_y\rangle = \langle l, m|\hat{L}_y|l, m\rangle = \frac{1}{2i}\left(\langle l, m|\hat{L}_+|l, m\rangle - \langle l, m|\hat{L}_-|l, m\rangle\right) = 0.$$

This is because $\hat{L}_+\,|l, m\rangle$ results in the orthogonal state $|l, m+1\rangle$, and $\hat{L}_-\,|l, m\rangle$ results in the orthogonal state $|l, m-1\rangle$, which are both orthogonal to $|l, m\rangle$.

$$\langle L_x\rangle = 0, \quad \langle L_y\rangle = 0.$$

b) We begin with the total angular momentum operator:

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2.$$

Taking the expectation value in the state $|l,m\rangle$, we have:

$$\langle l,m|\hat{L}^2|l,m\rangle = \hbar^2 l(l+1),$$

and

$$\langle l,m|\hat{L}_z^2|l,m\rangle = \hbar^2 m^2.$$

From the identity for $\hat{L}^2$, we can write:

$$\hbar^2 l(l+1) = \langle \hat{L}_x^2\rangle + \langle \hat{L}_y^2\rangle + \langle \hat{L}_z^2\rangle.$$

Substituting $\langle \hat{L}_z^2\rangle = \hbar^2 m^2$ into the equation:

$$\hbar^2 l(l+1) = \langle \hat{L}_x^2\rangle + \langle \hat{L}_y^2\rangle + \hbar^2 m^2.$$

Rearranging this gives:

$$\langle \hat{L}_x^2\rangle + \langle \hat{L}_y^2\rangle = \hbar^2(l(l+1) - m^2).$$

To proceed, we compute $\langle \hat{L}_x^2\rangle$ and $\langle \hat{L}_y^2\rangle$ separately. The operator $\hat{L}_x$ can be written in terms of the ladder operators as:

$$\hat{L}_x = \frac{1}{2}(L_+ + L_-).$$

$$\hat{L}_x^2 = \frac{1}{4}(L_+ + L_-)^2 = \frac{1}{4}(L_+^2 + L_-^2 + L_+L_- + L_-L_+).$$

Now, to compute the expectation value $\langle \hat{L}_x^2\rangle$, we use the action of the ladder operators on the states $|l,m\rangle$. The ladder operators L_+ and L_- act as:

$$L_+|l,m\rangle = \hbar\sqrt{(l-m)(l+m+1)}|l,m+1\rangle,$$

$$L_-|l,m\rangle = \hbar\sqrt{(l+m)(l-m+1)}|l,m-1\rangle.$$

Substituting these matrix elements into the expression for $\hat{L}_x^2$, we get:

$$\langle \hat{L}_x^2\rangle = \frac{1}{4}\left(\langle l,m|L_+^2|l,m\rangle + \langle l,m|L_-^2|l,m\rangle + \langle l,m|L_+L_-|l,m\rangle + \langle l,m|L_-L_+|l,m\rangle\right).$$

After simplifying, we obtain:

$$\langle \hat{L}_x^2\rangle = \frac{\hbar^2}{2}\left(l(l+1) - m^2\right)$$

Similarly, we compute $\langle \hat{L}_y^2\rangle$ using the corresponding expression for $\hat{L}_y$:

$$\hat{L}_y = \frac{1}{2i}(L_+ - L_-).$$

Following the same procedure, we find:

$$\langle \hat{L}_y^2\rangle = \frac{\hbar^2}{2}\left(l(l+1) - m^2\right)$$

Finally, adding the results for $\langle \hat{L}_x^2\rangle$ and $\langle \hat{L}_y^2\rangle$, we obtain:

$$\langle \hat{L}_x^2\rangle + \langle \hat{L}_y^2\rangle = \hbar^2(l(l+1) - m^2).$$

Therefore, the final result is:

$$\langle \hat{L}_x^2 \rangle = \langle \hat{L}_y^2 \rangle = \frac{\hbar^2}{2} \left(l(l+1) - m^2 \right).$$

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6) What is the expectation of the operator $\frac{1}{2}\left(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x\right)$ in the Y_l^m state?
Solution:
The operator

$$\frac{1}{2}\left(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x\right)$$

can be expressed in terms of the ladder operators $\hat{L}_+$ and $\hat{L}_-$. First, recall that:

$$\hat{L}_x = \frac{1}{2}\left(\hat{L}_+ + \hat{L}_-\right), \quad \hat{L}_y = \frac{1}{2i}\left(\hat{L}_+ - \hat{L}_-\right).$$

Substituting these into the operator:

$$\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x = \frac{1}{4i}\left((\hat{L}_+ + \hat{L}_-)(\hat{L}_+ - \hat{L}_-) + (\hat{L}_+ - \hat{L}_-)(\hat{L}_+ + \hat{L}_-)\right).$$

Expanding the products:

$$= \frac{1}{4i}\left(\hat{L}_+^2 - \hat{L}_-^2 + \hat{L}_+\hat{L}_- - \hat{L}_-\hat{L}_+ + \hat{L}_+^2 - \hat{L}_-^2 - \hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+\right).$$

Simplifying:

$$= \frac{1}{4i}\left(2(\hat{L}_+^2 - \hat{L}_-^2)\right).$$

Thus, the operator reduces to:

$$\frac{1}{2}\left(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x\right) = \frac{1}{2i}\left(\hat{L}_+^2 - \hat{L}_-^2\right).$$

Expectation Value in Y_l^m

The action of $\hat{L}_+$ and $\hat{L}_-$ on the state $|l,m\rangle$ is given by:

$$\hat{L}_+|l,m\rangle = \hbar\sqrt{(l-m)(l+m+1)}|l,m+1\rangle,$$
$$\hat{L}_-|l,m\rangle = \hbar\sqrt{(l+m)(l-m+1)}|l,m-1\rangle.$$

Applying $\hat{L}_+^2$ and $\hat{L}_-^2$ to $|l,m\rangle$, we get:

$$\hat{L}_+^2|l,m\rangle \propto |l,m+2\rangle, \quad \hat{L}_-^2|l,m\rangle \propto |l,m-2\rangle.$$

Since the states $|l,m+2\rangle$ and $|l,m-2\rangle$ are orthogonal to $|l,m\rangle$, their expectation values vanish:

$$\langle l,m|\hat{L}_+^2|l,m\rangle = 0, \quad \langle l,m|\hat{L}_-^2|l,m\rangle = 0.$$

Thus, the expectation value of the operator is:

$$\left\langle \frac{1}{2}\left(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x\right)\right\rangle = \frac{1}{2i}\left(\langle l,m|\hat{L}_+^2|l,m\rangle - \langle l,m|\hat{L}_-^2|l,m\rangle\right) = 0.$$

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7) A D_2 molecule at 30 K, at $t = 0$, is known to be in the state

$$\psi(\theta, \phi, 0) = \frac{3Y_1^1 + 4Y_7^3 + Y_7^1}{\sqrt{26}}.$$

a) What values of L and L_z will measurement find, and with what probabilities will these values occur?

b) What is $\psi(\theta, \phi, t)$?

c) What is $\langle E \rangle$ for the molecule at $t > 0$?

Energy levels E_l of the molecule is given by:

$$E_l = \hbar^2 \frac{l(l+1)}{2I},$$

where I is the moment of inertia of the molecule.

(Note: For the purely rotational states of D_2, assume that $\hbar/4\pi Ic = 30.4\ \text{cm}^{-1}$.)

Solution:

a) Given a superposition of spherical harmonic states, we must determine the possible values of L and L_z and their corresponding probabilities.

The given state is:

$$\psi(\theta, \phi, 0) = \frac{3Y_1^1 + 4Y_7^3 + Y_7^1}{\sqrt{26}}.$$

This is a linear combination of the spherical harmonics Y_1^1, Y_7^3, and Y_7^1.

Eigenvalues of $\hat{L}_z$: The eigenvalue of $\hat{L}_z$ for the state Y_l^m is $m\hbar$. The corresponding m values are:

- For Y_1^1, $m = 1$,
- For Y_7^3, $m = 3$,
- For Y_7^1, $m = 1$.

The probability of measuring a particular m is the square of the coefficient of the corresponding spherical harmonic. Therefore, the probabilities for each m are:

- For Y_1^1, the probability is $\left|\frac{3}{\sqrt{26}}\right|^2 = \frac{9}{26}$.
- For Y_7^3, the probability is $\left|\frac{4}{\sqrt{26}}\right|^2 = \frac{16}{26}$.
- For Y_7^1, the probability is $\left|\frac{1}{\sqrt{26}}\right|^2 = \frac{1}{26}$.

Thus, the possible values of L_z are:

$$L_z = m\hbar \quad \text{with probabilities:}$$

$$L_z = 1\hbar \quad (\text{probability: } \frac{9}{26} + \frac{1}{26} = \frac{10}{26}),$$
$$L_z = 3\hbar \quad (\text{probability: } \frac{16}{26}).$$

Possible Values of L:

The quantum number l determines the total angular momentum L. From the given spherical harmonics:

- For Y_1^1, $l = 1$,

- For Y_7^3 and Y_7^1, $l = 7$.

Thus, the possible values of L are:

$$L = \hbar\sqrt{l(l+1)} \quad \text{with } l = 1, 7.$$

The probabilities for each l are:

- $l = 1$ occurs with probability $\frac{9}{26}$,
- $l = 7$ occurs with probability $\frac{16+1}{26} = \frac{17}{26}$.

b) To find $\psi(\theta, \phi, t)$, we need to express the time evolution of the state. The time-dependent wavefunction is given by:

$$\psi(\theta, \phi, t) = \sum_{l,m} c_{lm} Y_l^m(\theta, \phi) e^{-iE_{lm}t/\hbar},$$

where c_{lm} are the coefficients in the expansion of the initial wavefunction.

For the given initial state, the time-dependent wavefunction is:

$$\psi(\theta, \phi, t) = \frac{3}{\sqrt{26}} Y_1^1 e^{-iE_1^1 t/\hbar} + \frac{4}{\sqrt{26}} Y_7^3 e^{-iE_7^3 t/\hbar} + \frac{1}{\sqrt{26}} Y_7^1 e^{-iE_7^1 t/\hbar}.$$

$$E_l = \hbar^2 \frac{l(l+1)}{2I},$$

c)The expectation value of the energy is given by:

$$\langle E \rangle = \sum_{l,m} |c_{lm}|^2 E_{lm}.$$

For the state $\psi(\theta, \phi, 0)$, we already have the coefficients c_{lm} and the corresponding energy eigenvalues. The energy expectation value is:

$$\langle E \rangle = \frac{9}{26} E_1 + \frac{16}{26} E_7 + \frac{1}{26} E_7,$$

where E_1 and E_7 are the energies for $l = 1$ and $l = 7$, respectively.

The energies are:

$$E_1 = \hbar^2 \frac{1(1+1)}{2I}, \quad E_7 = \hbar^2 \frac{7(7+1)}{2I}.$$

Using the given constant $\hbar/4\pi I c = 30.4\,\text{cm}^{-1}$, we can calculate $\langle E \rangle$.

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8) Consider a particle in a state described by

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

where N is a normalization factor.

(a) Show, by rewriting the $Y_1^{\pm 1.0}$ functions in terms of x, y, z, and r, that

$$Y_1^{\pm 1} = \mp \left(\frac{3}{4\pi}\right)^{1/2} \frac{x \pm iy}{2^{1/2} r}$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \frac{z}{r}$$

(b) Using this result, show that for a particle described by ψ above, $P\left(l_z = 0\right) = 2/3$, $P\left(l_z = +\hbar\right) = 1/6 = P\left(l_z = -\hbar\right)$.

Solution:

a) Definitions of Spherical Harmonics

The spherical harmonics for $l = 1$ are:

$$Y_1^1(\theta, \phi) = -\left(\frac{3}{8\pi}\right)^{1/2} e^{i\phi} \sin\theta,$$

$$Y_1^{-1}(\theta, \phi) = \left(\frac{3}{8\pi}\right)^{1/2} e^{-i\phi} \sin\theta,$$

$$Y_1^0(\theta, \phi) = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta.$$

<u>Convert to Cartesian Coordinates</u>

Using the relations:

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta,$$

and $r = \sqrt{x^2 + y^2 + z^2}$:

- For Y_1^1:

$$Y_1^1 = -\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{i\phi}.$$

  Substituting $\sin\theta e^{i\phi} = \frac{x+iy}{r}$:

$$Y_1^1 = -\left(\frac{3}{8\pi}\right)^{1/2} \frac{x+iy}{r}.$$

  Multiplying numerator and denominator by $\sqrt{2}$:

$$Y_1^1 = -\left(\frac{3}{4\pi}\right)^{1/2} \frac{x+iy}{\sqrt{2}r}.$$

- For Y_1^{-1}:

$$Y_1^{-1} = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{-i\phi}.$$

  Substituting $\sin\theta e^{-i\phi} = \frac{x-iy}{r}$:

$$Y_1^{-1} = \left(\frac{3}{8\pi}\right)^{1/2} \frac{x-iy}{r}.$$

  Multiplying numerator and denominator by $\sqrt{2}$:

$$Y_1^{-1} = \left(\frac{3}{4\pi}\right)^{1/2} \frac{x-iy}{\sqrt{2}r}.$$

- For Y_1^0:

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta.$$

  Substituting $\cos\theta = \frac{z}{r}$:

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \frac{z}{r}.$$

b) The wavefunction is given by:

$$\psi = N(x + y + 2z)e^{-ar}.$$

Using the spherical harmonic expansions:

$$\frac{x}{r} = \sqrt{\frac{2\pi}{3}}(-Y_1^1 + Y_1^{-1}), \quad \frac{y}{r} = i\sqrt{\frac{2\pi}{3}}(Y_1^1 + Y_1^{-1}), \quad \frac{z}{r} = \sqrt{\frac{4\pi}{3}}Y_1^0,$$

we rewrite:

$$x + y + 2z = r\left[\sqrt{\frac{2\pi}{3}}(-Y_1^1 + Y_1^{-1}) + i\sqrt{\frac{2\pi}{3}}(Y_1^1 + Y_1^{-1}) + 2\sqrt{\frac{4\pi}{3}}Y_1^0\right].$$

Grouping terms:

$$x + y + 2z = r\left(c_1 Y_1^1 + c_2 Y_1^{-1} + c_3 Y_1^0\right),$$

where the coefficients are:

$$c_1 = -\sqrt{\frac{2\pi}{3}} + i\sqrt{\frac{2\pi}{3}} = \sqrt{\frac{2\pi}{3}}(-1 + i),$$

$$c_2 = -\sqrt{\frac{2\pi}{3}} - i\sqrt{\frac{2\pi}{3}} = \sqrt{\frac{2\pi}{3}}(-1 - i),$$

$$c_3 = 2\sqrt{\frac{4\pi}{3}}.$$

<u>Normalization and Probabilities</u>
To find the probabilities, calculate the magnitudes:

$$|c_1|^2 = \left|\sqrt{\frac{2\pi}{3}}(-1 + i)\right|^2 = \frac{2\pi}{3} \times (1^2 + 1^2) = \frac{4\pi}{3},$$

$$|c_2|^2 = \left|\sqrt{\frac{2\pi}{3}}(-1 - i)\right|^2 = \frac{2\pi}{3} \times (1^2 + 1^2) = \frac{4\pi}{3},$$

$$|c_3|^2 = \left|2\sqrt{\frac{4\pi}{3}}\right|^2 = 4 \times \frac{4\pi}{3} = \frac{16\pi}{3}.$$

The sum of squares is:

$$\sum |c_m|^2 = |c_1|^2 + |c_2|^2 + |c_3|^2 = \frac{4\pi}{3} + \frac{4\pi}{3} + \frac{16\pi}{3} = \frac{24\pi}{3} = 8\pi.$$

The probabilities are:

$$P(l_z = +\hbar) = \frac{|c_1|^2}{\sum |c_m|^2} = \frac{\frac{4\pi}{3}}{8\pi} = \frac{1}{6},$$

$$P(l_z = -\hbar) = \frac{|c_2|^2}{\sum |c_m|^2} = \frac{\frac{4\pi}{3}}{8\pi} = \frac{1}{6},$$

$$P(l_z = 0) = \frac{|c_3|^2}{\sum |c_m|^2} = \frac{\frac{16\pi}{3}}{8\pi} = \frac{2}{3}.$$

Thus, the probabilities are:

$$P(l_z = 0) = \frac{2}{3}, \quad P(l_z = \pm\hbar) = \frac{1}{6}.$$