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# **Problem 6: Simultaneous Measurement of** $\hat{L}^2$ and $\hat{L}_x$

We need to determine whether the operators  $\hat{L}^2$  and  $\hat{L}_x$  can be measured simultaneously.

For two observables to be simultaneously measurable, their corresponding operators must commute. Thus, we need to check whether  $[\hat{L}^2, \hat{L}_x] = 0$ .

Let's calculate this commutator:

$$\begin{split} [\hat{L}^2, \hat{L}_x] &= \hat{L}^2 \hat{L}_x - \hat{L}_x \hat{L}^2 \\ \text{Since } \hat{L}^2 &= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \text{ we can write:} \\ [\hat{L}^2, \hat{L}_x] &= [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x] \end{split}$$

 $= [\hat{L}_x^2, \hat{L}_x] + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x]$ 

The first term  $[\hat{L}_x^2, \hat{L}_x] = 0$  since an operator commutes with itself and its powers.

For the remaining terms, we need the angular momentum commutation relations:  $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$ 

For  $[\hat{L}_{y}^{2}, \hat{L}_{x}]$ , we use the identity  $[A^{2}, B] = A[A, B] + [A, B]A$ :  $[\hat{L}_{y}^{2}, \hat{L}_{x}] = \hat{L}_{y}[\hat{L}_{y}, \hat{L}_{x}] + [\hat{L}_{y}, \hat{L}_{x}]\hat{L}_{y}$   $= \hat{L}_{y}(i\hbar\hat{L}_{z}) + (i\hbar\hat{L}_{z})\hat{L}_{y}$   $= i\hbar(\hat{L}_{y}\hat{L}_{z} + \hat{L}_{z}\hat{L}_{y})$ Similarly:  $[\hat{L}_{z}^{2}, \hat{L}_{x}] = \hat{L}_{z}[\hat{L}_{z}, \hat{L}_{x}] + [\hat{L}_{z}, \hat{L}_{x}]\hat{L}_{z}$   $= \hat{L}_{z}(-i\hbar\hat{L}_{y}) + (-i\hbar\hat{L}_{y})\hat{L}_{z}$   $= -i\hbar(\hat{L}_{z}\hat{L}_{y} + \hat{L}_{y}\hat{L}_{z})$ Therefore:  $[\hat{L}^{2}, \hat{L}_{x}] = 0 + i\hbar(\hat{L}_{y}\hat{L}_{z} + \hat{L}_{z}\hat{L}_{y}) - i\hbar(\hat{L}_{z}\hat{L}_{y} + \hat{L}_{y}\hat{L}_{z}) = 0$ 

This proves that  $[\hat{L}^2, \hat{L}_x] = 0$ , meaning that  $\hat{L}^2$  and  $\hat{L}_x$  can be measured simultaneously. The same would be true for  $\hat{L}^2$  and any component  $\hat{L}_i$ .

## Problem 16: Angle Between Angular Momentum Vector and z-axis

In classical mechanics, if we have a vector  $\vec{L}$  with a z-component  $L_z$ , the angle  $\theta$  between  $\vec{L}$  and the z-axis is given by:

 $\cos \theta = \frac{L_z}{|\vec{L}|}$ 

In quantum mechanics, we cannot specify the exact direction of the angular momentum vector due to the uncertainty principle. However, we can calculate the expectation value of  $\cos \theta$ :

$$\langle \cos \theta \rangle = \frac{\langle L_z \rangle}{\sqrt{\langle \hat{L}^2 \rangle}}$$

For an eigenstate of  $\hat{L}^2$  and  $\hat{L}_z$  with quantum numbers l and m, we have:  $\hat{L}^2|l,m\rangle = l(l+1)\hbar^2|l,m\rangle \ \hat{L}_z|l,m\rangle = m\hbar|l,m\rangle$ 

Therefore: 
$$\langle \cos \theta \rangle = \frac{m\hbar}{\sqrt{l(l+1)}\hbar} = \frac{m}{\sqrt{l(l+1)}}$$
  
For 3d orbitals,  $l = 2$ .

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Case 1:  $m = -2 \langle \cos \theta \rangle = \frac{-2}{\sqrt{2(2+1)}} = \frac{-2}{\sqrt{6}} = -\frac{2\sqrt{6}}{6} \approx -0.8165 \ \theta \approx$  $\cos^{-1}(-0.8165) \approx 144.7^{\circ}$ Case 2:  $m = +1 \langle \cos \theta \rangle = \frac{1}{\sqrt{2(2+1)}} = \frac{1}{\sqrt{6}} = \frac{\sqrt{6}}{6} \approx 0.4082 \ \theta \approx \cos^{-1}(0.4082) \approx$  $65.9^{\circ}$ 

#### **Problem 26:** Ionization Energy Calculation

The ionization energy is the energy required to remove an electron from a bound state to infinity (where the potential energy is zero).

For a hydrogen-like atom with nuclear charge Z, the energy of an electron

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in state *n* is:  $E_n = -\frac{Z^2 e^2}{8\pi\epsilon_0 a_0} \cdot \frac{1}{n^2} = -\frac{Z^2 Ry}{n^2}$ where  $Ry = \frac{e^2}{8\pi\epsilon_0 a_0} \approx 13.6$  eV is the Rydberg energy. The ionization energy for an electron in state *n* is:  $Z^2 Ry = \frac{Z^2 Ry}{Z^2 Ry} = \frac{Z^2 Ry}{Z^2 Ry}$  $I_n = E_{\infty} - E_n = 0 - \left(-\frac{Z^2 Ry}{n^2}\right) = \frac{Z^2 Ry}{n^2}$ For hydrogen (Z = 1): 1. 3s state (n = 3, l = 0):  $I_{3s} = \frac{Ry}{3^2} = \frac{13.6 \text{ eV}}{9} \approx 1.51 \text{ eV}$ 2. 4p state (n = 4, l = 1):  $I_{4p} = \frac{Ry}{4^2} = \frac{13.6 \text{ eV}}{16} \approx 0.85 \text{ eV}$ For multi-electron atoms, we would need to consider electron-electron in-

teractions and use effective nuclear charge or apply other quantum chemistry methods.

# Problem 39: Eigenvalue Problem for Orbital Magnetic Moment

The orbital magnetic moment operator is related to the angular momentum operator by:

 $\hat{\vec{\mu}}_l = -\frac{e}{2m_e}\vec{L}$ where e is the elementary charge and  $m_e$  is the electron mass.

The square of the orbital magnetic moment operator is:

$$\hat{\mu}_l^2 = \left(\frac{e}{2m_e}\right)^2 L^2$$

Since this is proportional to  $\hat{L}^2$ , they share the same eigenfunctions, which are the spherical harmonics  $Y_{lm}(\theta, \phi)$ .

The eigenvalue problem is:  $\hat{\mu}_l^2 \Psi_{nlm}(\vec{r}) = \mu_l^2 \Psi_{nlm}(\vec{r})$ where  $\Psi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\theta,\phi)$  are the hydrogen atom wavefunctions. The eigenvalues are:  $\mu_l^2 = (\frac{e}{2m_e})^2 l(l+1)\hbar^2 = (\frac{\mu_B}{\hbar})^2 l(l+1)\hbar^2 = \mu_B^2 l(l+1)$ where  $\mu_B = \frac{e\hbar}{2m_e}$  is the Bohr magneton.

Therefore, the eigenfunctions of  $\hat{\mu}_l^2$  are the hydrogen atom wavefunctions  $\Psi_{nlm}(\vec{r})$ , and the eigenvalues are  $\mu_B^2 l(l+1)$ .

### Problem 43: Second Order Approximation Equation Proof

We need to prove the equation:  $\sum_{k \neq n} |a_k^{(1)}|^2 + (a_n^{(2)*} + a_n^{(2)}) = 0$ This equation appears in time-independent perturbation theory. Let's start

with the normalization condition up to second order:

 $\langle \psi | \psi \rangle = 1$ 

Where  $|\psi\rangle = |\psi^{(0)}\rangle + \lambda |\psi^{(1)}\rangle + \lambda^2 |\psi^{(2)}\rangle + \dots$ 

If we expand  $|\psi\rangle$  in terms of the unperturbed eigenstates  $\{|n\rangle\}$ :

 $|\psi\rangle = \sum_{k} c_k |k\rangle$ 

where  $c_k = c_k^{(0)} + \lambda c_k^{(1)} + \lambda^2 c_k^{(2)} + \dots$ Assuming  $|\psi^{(0)}\rangle = |n\rangle$ , we have  $c_k^{(0)} = \delta_{kn}$ .

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The first-order coefficient  $c_k^{(1)}$  corresponds to  $a_k^{(1)}$  in the problem statement,

The instructure coefficient  $c_k$  corresponds to  $a_k$  in the problem statement, and similarly  $c_k^{(2)}$  corresponds to  $a_k^{(2)}$ . The normalization condition gives:  $\langle \psi | \psi \rangle = \sum_k |c_k|^2 = 1$ Expanding  $|c_k|^2$  to second order:  $|c_k|^2 = |c_k^{(0)} + \lambda c_k^{(1)} + \lambda^2 c_k^{(2)}|^2 + O(\lambda^3)$ For  $k \neq n$ ,  $c_k^{(0)} = 0$ , so:  $|c_k|^2 = |\lambda c_k^{(1)} + \lambda^2 c_k^{(2)}|^2 + O(\lambda^3) = \lambda^2 |c_k^{(1)}|^2 + O(\lambda^3)$ For k = n,  $c_n^{(0)} = 1$ , so:  $|c_n|^2 = |1 + \lambda c_n^{(1)} + \lambda^2 c_n^{(2)}|^2 + O(\lambda^3) = 1 + \lambda (c_n^{(1)*} + c_n^{(1)}) + \lambda^2 (|c_n^{(1)}|^2 + c_n^{(2)*} + c_n^{(2)}) + O(\lambda^3)$ 

Now, the normalization condition becomes:  $1 = \sum_{k \neq n} \lambda^2 |c_k^{(1)}|^2 + 1 + \lambda (c_n^{(1)*} + \lambda)^2 + \lambda (c_n^{(1)*} + \lambda (c_n^{(1)*} + \lambda)^2 + \lambda (c_n^{(1)*} + \lambda)^2 + \lambda (c_n^{(1)*} + \lambda (c_n^{(1)*} + \lambda)^2 + \lambda (c_n^{(1)*} + \lambda (c_n^{(1)*} + \lambda)^2 + \lambda (c_n^{(1)*} + \lambda)^2 + \lambda (c_n^{(1)*} + \lambda)^2 + \lambda (c_n^{(1)*} + \lambda (c_n^{(1)*} + \lambda)^2 + \lambda (c_n^{($  $c_n^{(1)}) + \lambda^2 (|c_n^{(1)}|^2 + c_n^{(2)*} + c_n^{(2)}) + O(\lambda^3)$ 

Comparing coefficients of  $\lambda$ :  $\lambda^1 : c_n^{(1)*} + c_n^{(1)} = 0$  (which means  $c_n^{(1)}$  is purely imaginary)

Comparing coefficients of  $\lambda^2$ :  $\sum_{k \neq n} |c_k^{(1)}|^2 + |c_n^{(1)}|^2 + c_n^{(2)*} + c_n^{(2)} = 0$ Since  $c_n^{(1)}$  is purely imaginary,  $|c_n^{(1)}|^2 = -c_n^{(1)*}c_n^{(1)} = 0$ Therefore:  $\sum_{k \neq n} |c_k^{(1)}|^2 + c_n^{(2)*} + c_n^{(2)} = 0$ 

Using the notation from the problem statement:  $\sum_{k \neq n} |a_k^{(1)}|^2 + (a_n^{(2)*} + a_n^{(2)*})^2$  $a_n^{(2)}) = 0$ 

This completes the proof.