## **Question 1:**

- (i) Write the conditions required for physical acceptability of wave function.
  - The wave function  $\psi(r,t)$  must satisfy the following conditions to be physically acceptable:
    - Single-valued: For every point in space and time, the wave function must have a unique value. This ensures a definite probability at any given point.
    - Finite: The wave function must be finite everywhere. If it were infinite at some point, it would imply an infinite probability of finding the particle at that point, which is physically impossible.
    - O Continuous: The wave function must be continuous everywhere. This means there are no abrupt jumps or breaks in the wave function.
    - Continuous First Derivatives: The first derivatives of the wave function with respect to position (\$\frac{\partialψ} {\partial x}\$, \$\frac{\partialψ} {\partial z}\$) must be continuous. This condition is necessary for the kinetic energy of the particle to be finite.
    - Square-integrable: The integral of the square of the modulus of the wave function over all space must be finite. This condition ensures that the wave function can be normalized, meaning the total probability of finding the particle somewhere in space is 1. Mathematically,  $\int |\psi(r,t)|^2 dV = 1$ .
- (ii) What are stationary states? Why are they called so?
  - Stationary States: Stationary states are the eigenstates of the Hamiltonian operator  $(\widehat{H})$  for a time-independent potential. They are solutions to the time-independent Schrödinger equation:  $\widehat{H}\psi(r) = E\psi(r)$ , where E is the energy eigenvalue.
  - Why they are called so: They are called "stationary" states because, for these states, the probability density  $|\psi(r,t)|^2$  is independent of time.

- O The full time-dependent wave function for a stationary state is given by  $\Psi(r,t) = \psi(r)e^{-iEt/\hbar}$ .
- 0 The probability density is  $|\Psi(r,t)|^2 = |\psi(r)e^{-iEt/\hbar}|^2 = |\psi(r)|^2 |e^{-iEt/\hbar}|^2 = |\psi(r)|^2 \cdot 1 = |\psi(r)|^2$ .
- o Since  $|\psi(r)|^2$  does not depend on time, the probability of finding the particle at any given position does not change with time. Therefore, any observable (like position, momentum, energy) that depends on the probability distribution will have time-independent expectation values. While the phase of the wave function evolves with time, the physical properties of the system remain constant.
- (iii) Let  $\psi_0(x)$  and  $\psi_2(x)$  are the ground state and second excited state energy eigenfunctions of a particle moving in a harmonic oscillator potential with frequency  $\omega$ . At t=0, the wavefunction of the particle is  $\psi(x,0)=1/\sqrt{3}\psi_0(x)+\psi_2(x)$ . Find  $\psi(x,t)$  for  $t\neq 0$ .
  - For a quantum harmonic oscillator, the energy eigenvalues are given by  $E_n = (n + 1/2)\hbar\omega$ .
  - Therefore, the energy of the ground state (n = 0) is  $E_0 = (0 + 1/2)\hbar\omega = \hbar\omega/2$ .
  - The energy of the second excited state (n = 2) is  $E_2 = (2 + 1/2)\hbar\omega = 5\hbar\omega/2$ .
  - The general time evolution of a stationary state eigenfunction  $\psi_n(x)$  is  $\psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar}$ .
  - Given the initial wavefunction at t = 0:  $\psi(x, 0) = \frac{1}{\sqrt{3}}\psi_0(x) + \psi_2(x)$ .
  - To find  $\psi(x,t)$  for  $t \neq 0$ , we apply the time evolution operator to each component of the superposition:  $\psi(x,t) = \frac{1}{\sqrt{3}} \psi_0(x) e^{-iE_0 t/\hbar} + \psi_2(x) e^{-iE_2 t/\hbar}$

- Substitute the energy eigenvalues:  $\psi(x,t) = \frac{1}{\sqrt{3}}\psi_0(x)e^{-i(\hbar\omega/2)t/\hbar} + \psi_2(x)e^{-i(5\hbar\omega/2)t/\hbar}\psi(x,t) = \frac{1}{\sqrt{3}}\psi_0(x)e^{-i\omega t/2} + \psi_2(x)e^{-i5\omega t/2}$
- (iv) List the four quantum numbers needed to describe an atomic electron? What is their physical significance?
  - The four quantum numbers needed to describe an atomic electron are:
    - a. Principal Quantum Number (n):
      - Physical Significance: It primarily determines the electron's energy level and the average distance of the electron from the nucleus. Higher values of *n* correspond to higher energy levels and larger average orbital radii. *n* can take positive integer values: 1,2,3,....
    - b. Angular Momentum (Azimuthal) Quantum Number (*l*):
      - Physical Significance: It determines the magnitude of the orbital angular momentum of the electron and the shape of the electron's orbital. For a given n, l can take integer values from 0 to n-1.
        - l = 0 (s subshell): spherical shape.
        - l = 1 (p subshell): dumbbell shape.
        - l = 2 (d subshell): more complex shapes (e.g., cloverleaf).
        - The magnitude of the orbital angular momentum is given by  $|L| = \sqrt{l(l+1)}\hbar$ .
    - c. Magnetic Quantum Number  $(m_l)$ :
      - Physical Significance: It determines the orientation of the orbital angular momentum vector in space, specifically its component along a chosen direction (conventionally the z-axis). For a given l,  $m_l$  can take integer values from -l to +l,

including 0. There are 2l + 1 possible values of  $m_l$  for each l. This quantizes the direction of the orbital.

- The z-component of orbital angular momentum is  $L_z = m_l \hbar$ .
- d. Spin Magnetic Quantum Number  $(m_s)$ :
  - Physical Significance: It describes the intrinsic angular momentum of the electron, called spin angular momentum. It's a fundamental property of the electron, similar to its charge and mass. Electrons behave as if they are spinning, creating a magnetic dipole moment.  $m_s$  can only take two values: +1/2 (spin up) or -1/2 (spin down).
    - The z-component of spin angular momentum is  $S_z = m_s \hbar$ .
- (v) For 6g state of hydrogen atom, what are the values of quantum number n, l,  $m_i$  and energy of the state?
  - Principal Quantum Number (n): The number "6" in "6g" directly indicates the principal quantum number. So, n = 6.
  - Angular Momentum Quantum Number (*l*): The letter "g" corresponds to a specific value of *l*. The correspondence is:

$$\circ$$
 s:  $l = 0$ 

o p: 
$$l = 1$$

o d: 
$$l = 2$$

o f: 
$$l = 3$$

o g: 
$$l = 4$$

o So, for a 6g state, l = 4.

- Magnetic Quantum Number  $(m_l)$ : For a given l,  $m_l$  can take any integer value from -l to +l.
  - o For l = 4,  $m_l$  can be -4, -3, -2, -1, 0, 1, 2, 3, 4. (Note: the question used  $m_l$ , which is a common typo for  $m_l$ ).
- Energy of the State  $(E_n)$ : For a hydrogen atom, the energy of a state depends only on the principal quantum number n. The formula is:  $E_n = -\frac{13.6}{n^2} \,\text{eV}$  For n = 6:  $E_6 = -\frac{13.6}{6^2} = -\frac{13.6}{36} \approx -0.3778 \,\text{eV}$ .

(vi) Compute the commutator  $[xp^2]$ .

- The commutator is defined as [A, B] = AB BA.
- We need to compute  $[x, p^2]$ .
- We can expand  $p^2$  as  $p \cdot p$ .
- Using the property [A, BC] = [A, B]C + B[A, C]:  $[x, p^2] = [x, p \cdot p] = [x, p]p + p[x, p]$ .
- We know the fundamental canonical commutation relation  $[x, p] = i\hbar$ .
- Substitute this into the expression:  $[x, p^2] = (i\hbar)p + p(i\hbar)[x, p^2] = i\hbar p + i\hbar p[x, p^2] = 2i\hbar p$ .

(vii) Show that (a)  $[L_x\hat{x}] = 0$  (b)  $[L_x\hat{y}] = i\hbar\hat{z}$ .

- The orbital angular momentum operator L is given by  $L = r \times p = (yp_z zp_y)\hat{\imath} + (zp_x xp_z)\hat{\jmath} + (xp_y yp_x)\hat{k}$ .
- Therefore, the component  $L_x = yp_z zp_y$ .
- Part (a):  $[L_x \hat{x}] = 0$ 
  - $\circ \ [L_x, \hat{x}] = [yp_z zp_y, \hat{x}]$
  - Using linearity of commutator:  $[yp_z, \hat{x}] [zp_y, \hat{x}]$
  - For the first term:  $[yp_z, \hat{x}] = y[p_z, \hat{x}] + [y, \hat{x}]p_z$ .

- We know  $[\hat{A}, \hat{B}] = 0$  if they are position coordinates or momentum coordinates with different indices, e.g., [y, x] = 0,  $[p_z, x] = 0$ .
- So,  $y[p_z, \hat{x}] = y \cdot 0 = 0$ .
- And  $[y, \hat{x}]p_z = 0 \cdot p_z = 0$ .
- Thus,  $[yp_z, \hat{x}] = 0$ .
- For the second term:  $[zp_y, \hat{x}] = z[p_y, \hat{x}] + [z, \hat{x}]p_y$ .
  - Similar to above,  $[p_y, \hat{x}] = 0$  and  $[z, \hat{x}] = 0$ .
  - Thus,  $[zp_v, \hat{x}] = 0$ .
- O Therefore,  $[L_x, \hat{x}] = 0 0 = 0$ .
- Part (b):  $[L_x \hat{y}] = i\hbar \hat{z}$ 
  - $\circ \ [L_x, \hat{y}] = [yp_z zp_y, \hat{y}]$
  - Using linearity:  $[yp_z, \hat{y}] [zp_y, \hat{y}]$
  - o For the first term:  $[yp_z, \hat{y}] = y[p_z, \hat{y}] + [y, \hat{y}]p_z$ .
    - We know  $[p_z, \hat{y}] = 0$  (different indices).
    - And  $[y, \hat{y}] = 0$  (coordinate with itself).
    - Thus,  $[yp_z, \hat{y}] = 0$ .
  - For the second term:  $[zp_y, \hat{y}] = z[p_y, \hat{y}] + [z, \hat{y}]p_y$ .
    - We know  $[p_y, \hat{y}] = -i\hbar$  (using  $[x_i, p_j] = i\hbar \delta_{ij}$ , so  $[p_y, y] = -i\hbar$ , and  $[y, p_y] = i\hbar$ ).
    - And  $[z, \hat{y}] = 0$  (different coordinates).
    - So,  $z[p_y, \hat{y}] = z(-i\hbar) = -i\hbar z$ .
    - And  $[z, \hat{y}]p_y = 0 \cdot p_y = 0$ .

- Thus,  $[zp_y, \hat{y}] = -i\hbar z$ .
- Therefore,  $[L_x, \hat{y}] = 0 (-i\hbar z) = i\hbar z$ .

## Question 2:

- (i) Solve the Schrodinger equation for a particle having energy  $E < V_0$  for a square well potential of finite depth  $V_0$ . Discuss the graphical representation of the transcendental equations.
  - Potential: The finite square well potential is defined as: V(x) = 0 for -a/2 < x < a/2 (Region II inside the well)  $V(x) = V_0$  for  $x \le -a/2$  and  $x \ge a/2$  (Region I and III outside the well) Here,  $V_0 > 0$ . We are looking for bound states, so the energy of the particle is  $0 < E < V_0$ .
  - Time-Independent Schrödinger Equation:  $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E V(x))\psi = 0$ .
  - Region I (x < -a/2):  $V(x) = V_0$ .  $\frac{d^2\psi}{dx^2} \frac{2m(V_0 E)}{\hbar^2} \psi = 0$ . Let  $\kappa^2 = \frac{2m(V_0 E)}{\hbar^2}$ . Since  $V_0 > E$ ,  $\kappa^2$  is positive. The equation becomes  $\frac{d^2\psi}{dx^2} \kappa^2\psi = 0$ . Solution:  $\psi_I(x) = Ae^{\kappa x} + Be^{-\kappa x}$ . For the wave function to be finite as  $x \to -\infty$ , B must be 0. So,  $\psi_I(x) = Ae^{\kappa x}$ .
  - Region II (-a/2 < x < a/2): V(x) = 0.  $\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$ . Let  $k^2 = \frac{2mE}{\hbar^2}$ . Since E > 0,  $k^2$  is positive. The equation becomes  $\frac{d^2\psi}{dx^2} + k^2\psi = 0$ . Solution:  $\psi_{II}(x) = C\sin(kx) + D\cos(kx)$ .
  - Region III (x > a/2):  $V(x) = V_0$ .  $\frac{d^2\psi}{dx^2} \kappa^2\psi = 0$ . Solution:  $\psi_{III}(x) = Fe^{\kappa x} + Ge^{-\kappa x}$ . For the wave function to be finite as  $x \to +\infty$ , F must be 0. So,  $\psi_{III}(x) = Ge^{-\kappa x}$ .
  - Applying Boundary Conditions: The wave function and its first derivative must be continuous at x = -a/2 and x = a/2.
    - $\circ$  At x = -a/2:

- i.  $\psi_I(-a/2) = \psi_{II}(-a/2) \Rightarrow Ae^{-\kappa a/2} = C\sin(-ka/2) + D\cos(-ka/2) = -C\sin(ka/2) + D\cos(ka/2)$ . (Eq. 1)
- ii.  $\psi_{I'}(-a/2) = \psi_{II'}(-a/2) \Rightarrow \kappa A e^{-\kappa a/2} = kC\cos(ka/2) + kD\sin(ka/2)$ . (Eq. 2)
- At x = a/2: 3.  $\psi_{II}(a/2) = \psi_{III}(a/2) \Rightarrow C\sin(ka/2) +$   $D\cos(ka/2) = Ge^{-\kappa a/2}$ . (Eq. 3) 4.  $\psi_{II'}(a/2) = \psi_{III'}(a/2) \Rightarrow$  $kC\cos(ka/2) - kD\sin(ka/2) = -\kappa Ge^{-\kappa a/2}$ . (Eq. 4)
- Solving for Even and Odd Parity Solutions:
  - The potential is symmetric (V(x) = V(-x)), so the eigenfunctions will have definite parity (even or odd).
  - Even solutions (symmetric):  $\psi_{II}(x) = D\cos(kx)$ . (Here, C = 0).
    - From (1):  $Ae^{-\kappa a/2} = D\cos(ka/2)$ .
    - From (2):  $\kappa A e^{-\kappa a/2} = kD\sin(ka/2)$ . (This should be  $\kappa A e^{-\kappa a/2} = -kD\sin(ka/2)$  due to the derivative of  $\cos(kx)$  being  $-k\sin(kx)$ ).
    - Let's restart with the correct derivatives for even solution  $(\psi_{II}(x) = D\cos(kx))$ :
      - $\psi_{II'}(x) = -kD\sin(kx)$ .
      - At x = -a/2:  $Ae^{-\kappa a/2} = D\cos(ka/2)$ .
      - $\kappa A e^{-\kappa a/2} = kD\sin(ka/2)$ . (using  $\sin(-ka/2) = -\sin(ka/2)$ ).
      - Dividing these two equations:  $\kappa = k \tan(k\alpha/2)$ . (Eq. A)
    - For x = a/2:
      - $D\cos(ka/2) = Ge^{-\kappa a/2}$ .
      - $-kD\sin(ka/2) = -\kappa Ge^{-\kappa a/2}$ .

- Dividing these two equations:  $k \tan(k\alpha/2) = \kappa$ . This is the same Eq. A.
- Odd solutions (anti-symmetric):  $\psi_{II}(x) = C\sin(kx)$ . (Here, D = 0).
  - Let's restart with the correct derivatives for odd solution  $(\psi_{II}(x) = C\sin(kx))$ :
    - $\psi_{II'}(x) = kC\cos(kx)$ .
    - At x = -a/2:  $Ae^{-\kappa a/2} = -C\sin(ka/2)$ .
    - $\kappa A e^{-\kappa a/2} = kC \cos(ka/2)$ .
    - Dividing these two equations:  $\kappa = -k\cot(k\alpha/2)$ . (Eq. B)
  - For x = a/2:

    - $C\sin(ka/2) = Ge^{-\kappa a/2}$ .  $kC\cos(ka/2) = -\kappa Ge^{-\kappa a/2}$ .
    - Dividing these two equations:  $k\cot(k\alpha/2) = -\kappa$ . This is the same Eq. B.
- Transcendental Equations:
  - $\circ$  Let Z = ka/2.
  - $\circ \text{ Also, } \kappa a/2 = \sqrt{\frac{2m(V_0 E)}{\hbar^2}} \frac{a}{2} = \sqrt{\frac{2mV_0}{\hbar^2} (\frac{a}{2})^2 \frac{2mE}{\hbar^2} (\frac{a}{2})^2} = \sqrt{Z_0^2 Z^2},$ where  $Z_0^2 = \frac{2mV_0}{k^2} (\frac{a}{2})^2$ .
  - For Even States:  $k \tan(k\alpha/2) = \kappa \Rightarrow Z \tan Z = \sqrt{Z_0^2 Z^2}$ .
  - For Odd States:  $-k\cot(k\alpha/2) = \kappa \Rightarrow -Z\cot Z = \sqrt{Z_0^2 Z^2}$ .
- **Graphical Representation:**

- O These equations are transcendental and cannot be solved analytically for Z (and hence E). They are solved graphically.
- $\circ$  Plot the left-hand side (LHS) and right-hand side (RHS) of each equation as functions of Z. The intersection points give the allowed values of Z.
- Let  $f(Z) = Z \tan Z$  and  $g(Z) = \sqrt{Z_0^2 Z^2}$  for even states.
- Let  $f'(Z) = -Z \cot Z$  and  $g(Z) = \sqrt{Z_0^2 Z^2}$  for odd states.
- The function  $g(Z) = \sqrt{Z_0^2 Z^2}$  represents a quarter circle of radius  $Z_0$  in the first quadrant (since Z must be positive, as E > 0). The possible values of Z are restricted to  $0 < Z < Z_0$ .
- For Even States  $(Z \tan Z = \sqrt{Z_0^2 Z^2})$ :
  - The graph of  $Z \tan Z$  consists of branches that start at 0, increase, and go to infinity as Z approaches  $(n + 1/2)\pi$  for integers n.
  - The intersections of these branches with the quarter circle g(Z) give the allowed energy values for the even states.
  - There is always at least one even bound state, regardless of the well's depth.
- For Odd States  $(-Z\cot Z = \sqrt{Z_0^2 Z^2})$ :
  - The graph of  $-Z\cot Z$  consists of branches that start at positive infinity and decrease to negative infinity as Z approaches  $n\pi$  for integers n.
  - The intersections of these branches with the quarter circle g(Z) give the allowed energy values for the odd states.
  - Odd states only exist if the well is deep enough. The first odd state appears when  $Z_0 > \pi/2$ .

(ii) Obtain the mathematical form of position operator in momentum space.

- In quantum mechanics, an operator can be represented in different bases (e.g., position space, momentum space).
- Position Space Representation:
  - o Position operator:  $\hat{x} = x$
  - $\circ \quad \text{Momentum operator: } \hat{p} = -i\hbar \frac{\partial}{\partial x}$
- Momentum Space Representation:
  - o Momentum operator:  $\hat{p} = p$
  - O We want to find the form of  $\hat{x}$  in momentum space.
- We use the Fourier transform relationship between a wave function in position space  $\psi(x)$  and its momentum space representation  $\phi(p)$ :  $\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx \ \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \phi(p) dp$
- Now, let's consider the action of the position operator  $\hat{x}$  on  $\psi(x)$  in position space:  $\hat{x}\psi(x) = x\psi(x)$
- To find the equivalent operator in momentum space, we transform  $x\psi(x)$  to momentum space:  $FT[x\psi(x)] = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} (x\psi(x)) dx$
- We can use the property that  $xe^{-ipx/\hbar} = i\hbar \frac{\partial}{\partial p} (e^{-ipx/\hbar})$ .
- So,  $\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} (i\hbar \frac{\partial}{\partial p} (e^{-ipx/\hbar})) \psi(x) dx$
- This can be written as  $i\hbar \frac{\partial}{\partial p} \left( \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx \right)$ .
- The expression in the parenthesis is simply  $\phi(p)$ .
- Therefore,  $FT[x\psi(x)] = i\hbar \frac{\partial}{\partial p} \phi(p)$ .

• This means that the position operator in momentum space is  $\hat{x} = i\hbar \frac{\partial}{\partial p}$ .

## Question 3:

The potential energy of a simple harmonic oscillator of mass m, oscillating with angular frequency  $\omega$  is  $V(x) = \frac{1}{2}m\omega^2x^2$ . (i) Write the time independent Schrodinger equation. Using the time independent schrodinger equation, evaluate the energy for the eigenstate  $\psi_0(ax) = \sqrt{(\alpha/\pi^{1/2})}e^{-a2x^2}$ ;  $\alpha = \sqrt{(m\omega/\hbar)}$  where  $\omega$  is the angular frequency of the oscillator.

- Time-Independent Schrödinger Equation: For a one-dimensional system, the time-independent Schrödinger equation is:  $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$  Substitute the given potential  $V(x) = \frac{1}{2}m\omega^2x^2$ :  $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x)$
- Evaluate Energy for given  $\psi_0(x)$ : Given  $\psi_0(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\alpha^2 x^2/2}$  (Note: The given  $\psi_0(ax)$  seems to have a typo with the exponent of e and the normalization factor. I'll use the standard ground state form for the harmonic oscillator which is  $\psi_0(x) = (\frac{\alpha}{\sqrt{\pi}})^{1/2} e^{-\alpha^2 x^2/2}$  where  $\alpha = \sqrt{m\omega/\hbar}$ . Let's assume the question meant  $\psi_0(x) = (\frac{\alpha}{\pi^{1/2}})^{1/2} e^{-\alpha^2 x^2/2}$ ). Let's re-read the exact form given in the question:  $\psi_0(ax) = \sqrt{(\alpha/\pi^{1/2})} e^{-a^2x^2}$ . This indicates the variable is ax. Let y = ax. Then  $\psi_0(y) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-y^2/2}$ . Then  $x = y/\alpha$ . This is an unusual notation. Assuming the common form of the ground state wavefunction where the variable in the exponential is  $(ax)^2/2$  or  $\alpha^2 x^2/2$ : Let's take the provided wavefunction as  $\psi_0(x) = \sqrt{\frac{\alpha}{\pi^{1/2}}} e^{-\alpha^2 x^2/2}$  (the  $\alpha$  in the exponential seems to be squared as  $a^2$  with a being  $\alpha$  from the question, and the term  $\frac{1}{2}$  is generally present for the ground state). We need to compute the second derivative of  $\psi_0(x)$ :  $\psi_0'(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\alpha^2 x^2/2} (-\alpha^2 x) \psi_0''(x) =$

# (ii) Find $\langle p \rangle$ for $\psi_0$ .

- The expectation value of momentum operator p is given by  $\langle p \rangle = \int_{-\infty}^{\infty} \psi_0^*(x) \hat{p} \psi_0(x) dx$ .
- The momentum operator in position space is  $\hat{p} = -i\hbar \frac{d}{dx}$ .
- We use the normalized ground state wavefunction  $\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\alpha^2 x^2/2}$ , where  $\alpha = \sqrt{m\omega/\hbar}$ .
- First, calculate  $\hat{p}\psi_0(x)$ :  $\hat{p}\psi_0(x) = -i\hbar \frac{d}{dx} \left[ \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\alpha^2 x^2/2} \right] \hat{p}\psi_0(x) = -i\hbar \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\alpha^2 x^2/2} (-\alpha^2 x) \hat{p}\psi_0(x) = i\hbar \alpha^2 x \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\alpha^2 x^2/2} = i\hbar \alpha^2 x \psi_0(x)$
- Now, calculate the expectation value:  $\langle p \rangle = \int_{-\infty}^{\infty} \psi_0^*(x) (i\hbar \alpha^2 x \psi_0(x)) dx$ Since  $\psi_0(x)$  is real,  $\psi_0^*(x) = \psi_0(x)$ .  $\langle p \rangle = i\hbar \alpha^2 \int_{-\infty}^{\infty} x |\psi_0(x)|^2 dx \langle p \rangle = i\hbar \alpha^2 \int_{-\infty}^{\infty} x \left(\frac{\alpha}{\sqrt{\pi}}\right) e^{-\alpha^2 x^2} dx$

- The integrand  $f(x) = xe^{-\alpha^2 x^2}$  is an odd function (because  $f(-x) = (-x)e^{-\alpha^2(-x)^2} = -xe^{-\alpha^2 x^2} = -f(x)$ ).
- The integral of an odd function over a symmetric interval (from  $-\infty$  to  $+\infty$ ) is zero.
- Therefore,  $\langle p \rangle = 0$ . This is expected for a particle in a bound state in a symmetric potential, as it has no net motion in one direction.
- (iii) If the harmonic oscillator is in the ground state at t=0, what will be the wavefunction at  $t = \pi/(2\omega)$ .
  - If the harmonic oscillator is in the ground state at t = 0, its initial wavefunction is  $\Psi(x, 0) = \psi_0(x)$ .
  - For a stationary state  $\psi_n(x)$  with energy  $E_n$ , the time-dependent wavefunction is  $\Psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar}$ .
  - For the ground state (n = 0), the energy is  $E_0 = \hbar \omega/2$ .
  - So,  $\Psi(x,t) = \psi_0(x)e^{-iE_0t/\hbar} = \psi_0(x)e^{-i(\hbar\omega/2)t/\hbar} = \psi_0(x)e^{-i\omega t/2}$ .
  - We need to find the wavefunction at  $t = \pi/(2\omega)$ .
  - Substitute  $t = \pi/(2\omega)$  into the expression:  $\Psi(x, t = \pi/(2\omega)) = \psi_0(x)e^{-i\omega(\pi/(2\omega))/2} \Psi(x, t = \pi/(2\omega)) = \psi_0(x)e^{-i\pi/4}$
  - Using Euler's formula  $e^{-i\theta} = \cos\theta i\sin\theta$ :  $e^{-i\pi/4} = \cos(\pi/4) i\sin(\pi/4) = \frac{1}{\sqrt{2}} i\frac{1}{\sqrt{2}}$ .
  - Therefore, the wavefunction at  $t = \pi/(2\omega)$  is:  $\Psi(x, \pi/(2\omega)) = \psi_0(x) \left(\frac{1}{\sqrt{2}} \frac{i}{\sqrt{2}}\right)$ .

## Question 4:

Write the Schrodinger equation for a 3D hydrogen atom in spherical polar coordinates. Derive three separate equations for r,  $\theta$ ,  $\phi$  using the method of separation of variables. Solve the equation for  $\theta$  to obtain the normalized eigenfunctions.

- Schrödinger Equation for 3D Hydrogen Atom in Spherical Polar Coordinates: The time-independent Schrödinger equation is  $\widehat{H}\psi = E\psi$ . For a hydrogen atom, the potential energy is  $V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$  (for hydrogen, Z=1). The Hamiltonian in spherical polar coordinates  $(r,\theta,\varphi)$  is:  $\widehat{H} = -\frac{\hbar^2}{2\mu} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right] + V(r)$  So, the Schrödinger equation is:  $-\frac{\hbar^2}{2\mu} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] + V(r)\psi = E\psi$
- Method of Separation of Variables: Assume the wavefunction can be separated into three functions, each depending on a single coordinate:  $\psi(r,\theta,\varphi) = R(r)\Theta(\theta)\Phi(\varphi) \text{ Substitute this into the Schrödinger equation}$  and multiply by  $\frac{2\mu r^2 \sin^2 \theta}{\hbar^2 R(r)\Theta(\theta)\Phi(\varphi)} \text{ to separate the terms: } \frac{\sin^2 \theta}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr}\right) + \frac{1}{\Theta \sin \theta} \frac{d\theta}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi} \frac{d^2 \Phi}{d\varphi^2} + \frac{2\mu r^2 \sin^2 \theta}{\hbar^2} (E V(r)) = 0 \text{ Rearrange the}$  equation to separate the  $\phi$  dependent term:  $\left[\frac{\sin^2 \theta}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr}\right) + \frac{1}{\Theta \sin \theta} \frac{d\Theta}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta}\right) + \frac{2\mu r^2 \sin^2 \theta}{\hbar^2} (E V(r))\right] = -\frac{1}{\Phi} \frac{d^2 \Phi}{d\varphi^2} \text{ Since the LHS}$  depends only on r and  $\theta$ , and the RHS depends only on  $\phi$ , both sides must be equal to a constant. Let this constant be  $m_L^2$ .
  - Equation for φ:  $\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m_l^2 \frac{d^2 \Phi}{d\phi^2} + m_l^2 \Phi = 0$  The solutions are  $\Phi(\varphi) = Ae^{im_l \varphi}$ . For  $\Phi(\varphi)$  to be single-valued,  $\Phi(\varphi + 2\pi) = \Phi(\varphi)$ , which implies  $e^{im_l 2\pi} = 1$ , so  $m_l$  must be an integer  $(m_l = 0, \pm 1, \pm 2, ...)$ . Normalized solution:  $\Phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im_l \varphi}$ .
  - o Now, substitute  $m_l^2$  back into the remaining equation and divide by  $\sin^2\theta: \frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu r^2}{\hbar^2}(E V(r)) = -\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{m_l^2}{\sin^2\theta}$
  - o Again, the LHS depends only on r, and the RHS depends only on  $\theta$ . Both sides must be equal to another constant. Let this constant be l(l+1).

- Equation for θ:  $\frac{1}{\sin\theta} \frac{d}{d\theta} \left( \sin\theta \frac{d\Theta}{d\theta} \right) \frac{m_l^2}{\sin^2\theta} \Theta + l(l+1)\Theta = 0$
- O Equation for r:  $\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} (E V(r)) R \frac{l(l+1)}{r^2} R = 0$
- Solve the equation for  $\theta$  to obtain the normalized eigenfunctions: The equation for  $\theta$  is the associated Legendre differential equation. Its solutions are the associated Legendre functions, which, when normalized, form part of the spherical harmonics  $Y_{l,m_l}(\theta,\varphi) = \Theta_{l,m_l}(\theta)\Phi_{m_l}(\varphi)$ . The solutions  $\Theta_{l,m_l}(\theta)$  are proportional to  $P_l^{|m_l|}(\cos\theta)$ , where  $P_l^m$  are associated Legendre polynomials. The normalized eigenfunctions for  $\Theta(\theta)$  are:  $\Theta_{l,m_l}(\theta) = \sqrt{\frac{(2l+1)}{2}\frac{(l-|m_l|)!}{(l+|m_l|)!}}P_l^{|m_l|}(\cos\theta)$  where  $P_l^{|m_l|}(\cos\theta)$  are the associated Legendre polynomials.
  - Conditions on l and  $m_l$ :
    - l must be a non-negative integer (l = 0,1,2,...). This comes from the requirement that the series solution for  $\Theta(\theta)$  terminates.
    - $m_l$  must be an integer and  $|m_l| \le l$ . This ensures the solutions are well-behaved.
  - Examples of  $\Theta_{l,m_l}(\theta)$ :

• 
$$l = 0, m_l = 0: \Theta_{0,0}(\theta) = \sqrt{1/2}P_0^0(\cos\theta) = \sqrt{1/2} \cdot 1 = \sqrt{1/2}$$

• 
$$l = 1, m_l = 0: \Theta_{1,0}(\theta) = \sqrt{3/2}P_1^0(\cos\theta) = \sqrt{3/2}\cos\theta$$

• 
$$l = 1, m_l = \pm 1$$
:  $\Theta_{1,+1}(\theta) = \sqrt{3/4}P_1^1(\cos\theta) = \sqrt{3/4}\sin\theta$ 

• 
$$l = 2, m_l = 0: \Theta_{2,0}(\theta) = \sqrt{5/8}P_2^0(\cos\theta) = \sqrt{5/8}(3\cos^2\theta - 1)$$

• 
$$l = 2, m_l = \pm 1$$
:  $\Theta_{2,\pm 1}(\theta) = \sqrt{15/8}P_2^1(\cos\theta) = \sqrt{15/8}\sin\theta\cos\theta$ 

• 
$$l = 2, m_l = \pm 2$$
:  $\Theta_{2,\pm 2}(\theta) = \sqrt{15/32}P_2^2(\cos\theta) = \sqrt{15/32}\sin^2\theta$ 

## Question 5:

- (i) What is spin angular momentum? Discuss the experimental observations which could not be accounted for without introducing the spin angular momentum.
  - Spin Angular Momentum: Spin angular momentum is an intrinsic form of angular momentum carried by elementary particles, composite particles (like protons and neutrons), and nuclei. It is a fundamental property, similar to mass and charge, and is not associated with the actual spatial motion of the particle. Although often described as a "spin" like a classical object rotating, it is a purely quantum mechanical phenomenon with no classical analogue. For an electron, the magnitude of its spin angular momentum is fixed at S = √s(s+1)ħ, where s is the spin quantum number (s = 1/2 for electrons). Its z-component is quantized to Sz = msħ, where ms = ±1/2.
  - Experimental Observations that Required Spin Angular Momentum:
    - e. Stern-Gerlach Experiment (1922):
      - Observation: When a beam of neutral silver atoms (which have a single unpaired electron in their outermost shell, so their net orbital angular momentum is zero) was passed through an inhomogeneous magnetic field, it split into two distinct beams, not into 2l + 1 components as predicted by orbital angular momentum quantization (which would have been one unsplit beam for l = 0).
      - Explanation (with spin): This experiment provided direct evidence for space quantization and, more importantly, for the existence of an intrinsic angular momentum (spin) of the electron. The two beams corresponded to the two possible spin orientations ( $m_s = +1/2$  and  $m_s = -1/2$ ) of the electron in the magnetic field. Without spin, the atoms with zero orbital

angular momentum should have shown no deflection or an unsplit beam.

# f. Fine Structure of Atomic Spectra:

- Observation: High-resolution atomic spectra revealed that many spectral lines, previously thought to be single, were actually closely spaced doublets or triplets (e.g., the sodium D-lines). This splitting could not be fully explained by the relativistic corrections to the Schrödinger equation or by the interaction of orbital angular momentum with the magnetic field.
- Explanation (with spin): This fine structure is explained by the spin-orbit coupling. The electron's intrinsic magnetic dipole moment (due to its spin) interacts with the magnetic field generated by its orbital motion around the nucleus. This interaction leads to a slight splitting of energy levels, which in turn causes the observed fine structure in the spectral lines.

# g. Anomalous Zeeman Effect:

- Observation: When atomic spectral lines are observed in the presence of an external magnetic field, they split into multiple components. The "normal" Zeeman effect, predicted by classical physics, applied only to certain spectral lines and predicted a simple splitting pattern. However, for most atoms, the splitting pattern was more complex, showing a different number of components or different spacings than the normal Zeeman effect.
- Explanation (with spin): The anomalous Zeeman effect is explained by considering both the orbital angular momentum and the spin angular momentum of the electrons, and their interaction with the external magnetic field. The total magnetic moment is a sum of contributions from both orbital and spin angular momenta, leading to more complex splitting patterns

that require the introduction of the Landé g-factor and the concept of electron spin.

# h. Pauli Exclusion Principle:

- Observation: Experimental observations of electron configurations in atoms showed that no two electrons in an atom could occupy the exact same quantum state.
- Explanation (with spin): Wolfgang Pauli formulated the Pauli Exclusion Principle, which states that no two identical fermions (like electrons) can occupy the same quantum state simultaneously. This principle necessarily included the spin quantum number  $(m_s)$  as one of the four quantum numbers defining a state. Without spin, the principle would not adequately explain the observed electron shell structure and the chemical properties of elements.
- (ii) What are Pauli Spin matrices. For  $s = \frac{1}{2}$ , obtain the matrix form of  $S_z$ .
  - Pauli Spin Matrices: Pauli spin matrices  $(\sigma_x, \sigma_y, \sigma_z)$  are a set of three  $2 \times 2$  complex Hermitian matrices that are fundamental in the quantum mechanical description of spin-1/2 particles, such as electrons. They are proportional to the components of the spin angular momentum operator. They satisfy specific commutation relations and are used to represent the spin angular momentum operators in matrix form in the spin-1/2 basis. The matrices are:  $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
  - Matrix Form of  $S_z$  for  $s=\frac{1}{2}$ : The spin angular momentum operator S is related to the Pauli spin matrices by  $S=\frac{\hbar}{2}\sigma$ . Therefore, the components are:  $S_x=\frac{\hbar}{2}\sigma_x=\frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}S_y=\frac{\hbar}{2}\sigma_y=\frac{\hbar}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix}S_z=\frac{\hbar}{2}\sigma_z=\frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$  The matrix form of  $S_z$  for s=1/2 is:  $S_z=\begin{pmatrix}\hbar/2&0\\0&-\hbar/2\end{pmatrix}$  This matrix acts on a two-component spin state (spinor)  $\alpha \choose \beta$ , where  $\alpha$  corresponds to spin-up  $\alpha \choose \beta=+1/2$  and  $\beta$  corresponds to spin-down  $\alpha \choose \beta=-1/2$ .

- (iii) What is total angular momentum? After defining ladder operator  $J_+$  and  $J_-$  obtain (a)  $[J_+J_-]$  (b)  $[J_+J_z]$ .
  - Total Angular Momentum: In quantum mechanics, the total angular momentum (J) of a particle or a system is the sum of its orbital angular momentum (L) and its spin angular momentum (S): J = L + S For a system of multiple particles, it is the vector sum of the total orbital angular momentum and the total spin angular momentum of all particles. The components of J (J<sub>x</sub>,J<sub>y</sub>,J<sub>z</sub>) satisfy the same commutation relations as L and S: [J<sub>x</sub>,J<sub>y</sub>] = iħJ<sub>z</sub> [J<sub>y</sub>,J<sub>z</sub>] = iħJ<sub>x</sub> [J<sub>z</sub>,J<sub>x</sub>] = iħJ<sub>y</sub> Also, [J<sup>2</sup>,J<sub>x</sub>] = [J<sup>2</sup>,J<sub>y</sub>] = [J<sup>2</sup>,J<sub>y</sub>] = [J<sup>2</sup>,J<sub>y</sub>] = [J<sup>2</sup>,J<sub>y</sub>] = 0, where J<sup>2</sup> = J<sub>x</sub><sup>2</sup> + J<sub>y</sub><sup>2</sup> + J<sub>z</sub><sup>2</sup>.
  - Ladder Operators  $(J_+ \text{ and } J_-)$ : The ladder (or raising/lowering) operators for total angular momentum are defined as:  $J_+ = J_x + iJ_y$  (raising operator)  $J_- = J_x iJ_y$  (lowering operator) They are used to move between different  $m_i$  eigenstates for a given j.
  - Derivations: (a)  $[J_+J_-]$ :  $[J_+,J_-] = [J_x + iJ_y,J_x iJ_y]$  Using linearity and properties of commutators:  $= [J_x,J_x] [J_x,iJ_y] + [iJ_y,J_x] [iJ_y,iJ_y] = 0 i[J_x,J_y] + i[J_y,J_x] i^2[J_y,J_y] = -i(i\hbar J_z) + i(-i\hbar J_z) (-1) \cdot 0 = -i^2\hbar J_z i^2\hbar J_z = \hbar J_z + \hbar J_z = 2\hbar J_z$  So,  $[J_+J_-] = 2\hbar J_z$ . (b)  $[J_+J_z]$ :  $[J_+,J_z] = [J_x + iJ_y,J_z]$  Using linearity:  $= [J_x,J_z] + i[J_y,J_z]$  We know  $[J_x,J_z] = -i\hbar J_y$  (from  $[J_z,J_x] = i\hbar J_y$ ) And  $[J_y,J_z] = i\hbar J_x$  Substitute these:  $= (-i\hbar J_y) + i(i\hbar J_x) = -i\hbar J_y + i^2\hbar J_x = -i\hbar J_y \hbar J_x = -\hbar (J_x + iJ_y) = -\hbar J_+$  So,  $[J_+J_z] = -\hbar J_+$ .

# Question 6:

- (i) Find  $\langle r \rangle$  and  $\langle r^2 \rangle$  for an electron in the ground state of the hydrogen atom? Express the answer in terms of Bohr radius.
  - Ground State Wavefunction of Hydrogen Atom  $(n=1, l=0, m_l=0)$ :  $\psi_{100}(r, \theta, \varphi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \text{ where } a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \text{ is the Bohr radius.}$

• Expectation Value of  $r(\langle r \rangle)$ :  $\langle r \rangle = \int \psi_{100}^* r \psi_{100} dV$  In spherical polar coordinates,  $dV = r^2 \sin\theta dr d\theta d\phi$ .  $\langle r \rangle =$ 

$$\int_{0}^{\infty} \int_{0}^{\pi} \int_{0}^{2\pi} \left( \frac{1}{\sqrt{\pi a_{0}^{3}}} e^{-r/a_{0}} \right)^{*} r \left( \frac{1}{\sqrt{\pi a_{0}^{3}}} e^{-r/a_{0}} \right) r^{2} \sin\theta dr d\theta d\phi \langle r \rangle = \frac{1}{\pi a_{0}^{3}} \int_{0}^{\infty} r^{3} e^{-2r/a_{0}} dr \int_{0}^{\pi} \sin\theta d\theta \int_{0}^{2\pi} d\phi$$

- 0 The angular integrals are standard:  $\int_0^{\pi} \sin \theta d\theta = [-\cos \theta]_0^{\pi} = -(-1) (-1) = 2 \int_0^{2\pi} d\phi = 2\pi$
- o For the radial integral, use the definite integral formula:

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}. \text{ Here, } n = 3 \text{ and } a = 2/a_0.$$

$$\int_0^\infty r^3 e^{-2r/a_0} dr = \frac{3!}{(2/a_0)^{3+1}} = \frac{6}{(2/a_0)^4} = \frac{6}{16/a_0^4} = \frac{6a_0^4}{16} = \frac{3}{8}a_0^4.$$

- O Substitute these results back into  $\langle r \rangle$ :  $\langle r \rangle = \frac{1}{\pi a_0^3} \left(\frac{3}{8} a_0^4\right) (2) (2\pi) \langle r \rangle = \frac{1}{\pi a_0^3} \frac{3}{8} a_0^4 \cdot 4\pi = \frac{12\pi a_0^4}{8\pi a_0^3} = \frac{3}{2} a_0.$
- $\circ \quad \text{So, } \langle r \rangle = \frac{3}{2} a_0.$
- Expectation Value of  $r^2$  ( $\langle r^2 \rangle$ ):  $\langle r^2 \rangle = \int \psi_{100}^* r^2 \psi_{100} dV \langle r^2 \rangle = \frac{1}{\pi a_0^3} \int_0^\infty r^4 e^{-2r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi$ 
  - The angular integrals are the same:  $2 \cdot 2\pi = 4\pi$ .
  - o For the radial integral, n = 4 and  $a = 2/a_0$ .  $\int_0^\infty r^4 e^{-2r/a_0} dr = \frac{4!}{(2/a_0)^{4+1}} = \frac{24}{(2/a_0)^5} = \frac{24}{32/a_0^5} = \frac{24a_0^5}{32} = \frac{3}{4}a_0^5.$
  - O Substitute these results back into  $\langle r^2 \rangle$ :  $\langle r^2 \rangle = \frac{1}{\pi a_0^3} \left( \frac{3}{4} a_0^5 \right) (4\pi) \langle r^2 \rangle = \frac{12\pi a_0^5}{4\pi a_0^3} = 3a_0^2$ .
  - $\circ$  So,  $\langle r^2 \rangle = 3a_0^2$ .

- (ii) At a given instant of time, a system is in the state  $Y(\theta, \varphi) = \sqrt{3/4\pi} \sin\theta \sin\varphi$ . Determine the expectation values of  $L_z$  and  $L^2$ .
  - The given state is an angular wavefunction  $Y(\theta, \varphi)$ . This is a spherical harmonic.
  - We know that spherical harmonics are eigenfunctions of  $L^2$  and  $L_z$ .  $L^2 Y_{l,m_l}(\theta,\varphi) = l(l+1)\hbar^2 Y_{l,m_l}(\theta,\varphi) L_z Y_{l,m_l}(\theta,\varphi) = m_l \hbar Y_{l,m_l}(\theta,\varphi)$
  - We need to express the given  $Y(\theta, \varphi)$  in terms of standard spherical harmonics  $Y_{l,m_l}(\theta, \varphi)$ . The standard spherical harmonics are:  $Y_{1,1}(\theta, \varphi) = -\sqrt{3/8\pi}\sin\theta e^{i\phi} Y_{1,0}(\theta, \varphi) = \sqrt{3/4\pi}\cos\theta Y_{1,-1}(\theta, \varphi) = \sqrt{3/8\pi}\sin\theta e^{-i\phi}$
  - We have  $Y(\theta, \varphi) = \sqrt{3/4\pi} \sin\theta \sin\phi$ .
  - We know  $\sin \phi = \frac{e^{i\phi} e^{-i\phi}}{2i}$ .
  - So,  $Y(\theta, \varphi) = \sqrt{3/4\pi} \sin\theta \frac{e^{i\phi} e^{-i\phi}}{2i} Y(\theta, \varphi) = \frac{1}{2i} \sqrt{3/4\pi} \sin\theta e^{i\phi} \frac{1}{2i} \sqrt{3/4\pi} \sin\theta e^{-i\phi} Y(\theta, \varphi) = \frac{1}{2i} \left( -\sqrt{2}Y_{1,1} \right) \frac{1}{2i} \left( \sqrt{2}Y_{1,-1} \right)$  (multiplying the Y\_1,1 and Y\_1,-1 by  $\sqrt{8\pi/3}$  and extracting  $\sin\theta e^{i\phi}$  and  $\sin\theta e^{-i\phi}$ )  $Y(\theta, \varphi) = \frac{\sqrt{2}}{2i} \left( -Y_{1,1} Y_{1,-1} \right) Y(\theta, \varphi) = \frac{i\sqrt{2}}{2} \left( Y_{1,1} + Y_{1,-1} \right) Y(\theta, \varphi) = \frac{i}{\sqrt{2}} \left( Y_{1,1} + Y_{1,-1} \right)$
  - Normalization Check:  $|Y(\theta, \varphi)|^2 = |\frac{i}{\sqrt{2}}(Y_{1,1} + Y_{1,-1})|^2 = \frac{1}{2}(|Y_{1,1}|^2 + |Y_{1,-1}|^2 + Y_{1,1}^*Y_{1,-1} + Y_{1,1}Y_{1,-1}^*)$ . Since  $Y_{l,m_l}$  are orthonormal,  $\int Y_{l,m_l}^* Y_{l',m_{l'}} d\Omega = \delta_{ll'} \delta_{m_l m_{l'}}. \int |Y(\theta, \varphi)|^2 d\Omega = \frac{1}{2}(\int |Y_{1,1}|^2 d\Omega + \int |Y_{1,-1}|^2 d\Omega + \text{cross-terms that vanish}) = \frac{1}{2}(1+1) = 1$ . The given state is normalized.
  - Expectation Value of  $L_z$  ( $\langle L_z \rangle$ ):  $\langle L_z \rangle = \int Y^*(\theta, \varphi) L_z Y(\theta, \varphi) d\Omega L_z Y_{1,1} = 1\hbar Y_{1,1} L_z Y_{1,-1} = -1\hbar Y_{1,-1} L_z Y(\theta, \varphi) = L_z \left[ \frac{i}{\sqrt{2}} (Y_{1,1} + Y_{1,-1}) \right] = \frac{i}{\sqrt{2}} (L_z Y_{1,1} + L_z Y_{1,-1}) L_z Y(\theta, \varphi) = \frac{i}{\sqrt{2}} (\hbar Y_{1,1} \hbar Y_{1,-1}) = \frac{i\hbar}{\sqrt{2}} (Y_{1,1} Y_{1,-1})$

Now, integrate: 
$$\langle L_z \rangle = \int \left[ \frac{i}{\sqrt{2}} (Y_{1,1} + Y_{1,-1}) \right]^* \left[ \frac{i\hbar}{\sqrt{2}} (Y_{1,1} - Y_{1,-1}) \right] d\Omega \ \langle L_z \rangle = \frac{1}{2} \int (-i) (Y_{1,1}^* + Y_{1,-1}^*) (i\hbar) (Y_{1,1} - Y_{1,-1}) d\Omega \ \langle L_z \rangle = \frac{\hbar}{2} \int (Y_{1,1}^* + Y_{1,-1}^*) (Y_{1,1} - Y_{1,-1}^*) d\Omega \ \langle L_z \rangle = \frac{\hbar}{2} \int (Y_{1,1}^* Y_{1,1} - Y_{1,1}^* Y_{1,-1} + Y_{1,-1}^* Y_{1,1} - Y_{1,-1}^* Y_{1,-1}) d\Omega \ \text{Using}$$
 orthonormality:  $\langle L_z \rangle = \frac{\hbar}{2} (1 - 0 + 0 - 1) = \frac{\hbar}{2} (0) = 0$ . So,  $\langle L_z \rangle = 0$ .

• Expectation Value of  $L^2$  ( $\langle L^2 \rangle$ ):  $\langle L^2 \rangle = \int Y^*(\theta, \varphi) L^2 Y(\theta, \varphi) d\Omega \ L^2 Y_{1,1} = 1(1+1)\hbar^2 Y_{1,1} = 2\hbar^2 Y_{1,1} \ L^2 Y_{1,-1} = 1(1+1)\hbar^2 Y_{1,-1} = 2\hbar^2 Y_{1,-1}$   $L^2 Y(\theta, \varphi) = L^2 \left[ \frac{i}{\sqrt{2}} (Y_{1,1} + Y_{1,-1}) \right] = \frac{i}{\sqrt{2}} (L^2 Y_{1,1} + L^2 Y_{1,-1}) \ L^2 Y(\theta, \varphi) = \frac{i}{\sqrt{2}} (2\hbar^2 Y_{1,1} + 2\hbar^2 Y_{1,-1}) = 2\hbar^2 \frac{i}{\sqrt{2}} (Y_{1,1} + Y_{1,-1}) = 2\hbar^2 Y(\theta, \varphi) \text{ Now,}$  integrate:  $\langle L^2 \rangle = \int Y^*(\theta, \varphi) [2\hbar^2 Y(\theta, \varphi)] d\Omega \ \langle L^2 \rangle = 2\hbar^2 \int |Y(\theta, \varphi)|^2 d\Omega$ Since  $Y(\theta, \varphi)$  is normalized,  $\int |Y(\theta, \varphi)|^2 d\Omega = 1$ . Therefore,  $\langle L^2 \rangle = 2\hbar^2$ .

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