

UPSC PHYSICS PYQ SOLUTION

Quantum Mechanics - Part 5

Contents

| | |
|---|----|
| 51 Show that the Pauli spin matrices satisfy the following: | 2 |
| 52 The normalized wave function for the electron in hydrogen atom for the ground state is $\psi(r) = (\pi a_0^3)^{-1/2} \exp\left(\frac{-r}{a_0}\right)$ where a_0 is the radius of the first Bohr orbit. Show that the most probable position of the electron is a_0 . | 4 |
| 53 Let $\vec{\sigma}$ be the vector operator with components equal to Pauli's spin matrices $\sigma_x, \sigma_y, \sigma_z$. If \vec{a} and \vec{b} are vectors in 3D space, prove the identity $(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\sigma} \cdot (\vec{a} \times \vec{b})$. | 6 |
| 54 The normalized wave function for the electron in the ground state of the hydrogen atom is given by $\psi(r) = \frac{1}{(\pi a_0^3)^{1/2}} e^{-r/a_0}$ where a_0 is the radius of the first Bohr orbit. Calculate $\langle r \rangle$ and $\langle \frac{1}{r} \rangle$. | 8 |
| 55 Using the definition $\vec{L} = \vec{r} \times \vec{p}$ of the orbital angular momentum operator, evaluate $[L_x, L_y]$. | 11 |
| 56 Calculate the probability of finding the electron within a distance r_0 of the proton in the ground state. | 13 |
| 57 If \hat{x} and \hat{p} are the position and momentum operators, prove the commutation relation $[\hat{p}^2, \hat{x}] = -2i\hbar\hat{p}$ | 15 |
| 58 Write down Pauli spin matrices. Express J_x, J_y , and J_z in terms of Pauli spin matrices. | 16 |
| 59 Using the commutation relations $[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$, deduce the commutation relation between the components of angular momentum operator \mathbf{L} . | 17 |
| 60 Solve the Schrödinger equation for a particle in a three-dimensional rectangular potential barrier. Explain the terms degenerate and non-degenerate states in this context. | 19 |

51 Show that the Pauli spin matrices satisfy the following:

1. $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$
2. $\sigma_x \sigma_y = -\sigma_y \sigma_x = i\sigma_z$
3. $\sigma_y \sigma_z = -\sigma_z \sigma_y = i\sigma_x$
4. $\sigma_z \sigma_x = -\sigma_x \sigma_z = i\sigma_y$

Introduction:

The Pauli spin matrices σ_x , σ_y , and σ_z are fundamental operators in quantum mechanics, particularly in the description of spin- $\frac{1}{2}$ particles. These matrices not only obey specific algebraic properties but also play a critical role in the representation of angular momentum in quantum mechanics. The matrices are defined as follows:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Solution:

We need to verify that the following properties hold for the Pauli matrices:

1. $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$
2. $\sigma_x \sigma_y = -\sigma_y \sigma_x = i\sigma_z$
3. $\sigma_y \sigma_z = -\sigma_z \sigma_y = i\sigma_x$
4. $\sigma_z \sigma_x = -\sigma_x \sigma_z = i\sigma_y$

Step 1: Verify that $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$.

Calculate σ_x^2 :

$$\sigma_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

Similarly, calculate σ_y^2 :

$$\sigma_y^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

And calculate σ_z^2 :

$$\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

Thus, $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$.

Step 2: Verify that $\sigma_x \sigma_y = -\sigma_y \sigma_x = i\sigma_z$.

Calculate $\sigma_x \sigma_y$:

$$\sigma_x \sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\sigma_z$$

Now, calculate $\sigma_y\sigma_x$:

$$\sigma_y\sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i\sigma_z$$

This confirms that $\sigma_x\sigma_y = -\sigma_y\sigma_x = i\sigma_z$.

Step 3: Verify that $\sigma_y\sigma_z = -\sigma_z\sigma_y = i\sigma_x$.

Calculate $\sigma_y\sigma_z$:

$$\sigma_y\sigma_z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i\sigma_x$$

Now, calculate $\sigma_z\sigma_y$:

$$\sigma_z\sigma_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = -i\sigma_x$$

This confirms that $\sigma_y\sigma_z = -\sigma_z\sigma_y = i\sigma_x$.

Step 4: Verify that $\sigma_z\sigma_x = -\sigma_x\sigma_z = i\sigma_y$.

Calculate $\sigma_z\sigma_x$:

$$\sigma_z\sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_y$$

Now, calculate $\sigma_x\sigma_z$:

$$\sigma_x\sigma_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i\sigma_y$$

This confirms that $\sigma_z\sigma_x = -\sigma_x\sigma_z = i\sigma_y$.

Conclusion:

These commutation and anti-commutation relations are crucial in understanding the behavior of spin- $\frac{1}{2}$ systems and are widely applicable in various quantum systems.

52 The normalized wave function for the electron in hydrogen atom for the ground state is $\psi(r) = (\pi a_0^3)^{-1/2} \exp\left(\frac{-r}{a_0}\right)$ where a_0 is the radius of the first Bohr orbit. Show that the most probable position of the electron is a_0 .

Introduction:

In quantum mechanics, the probability density of finding a particle at a particular position r is given by $|\psi(r)|^2$. For a spherically symmetric system, the probability of finding the electron in a thin shell of radius r and thickness dr is proportional to $|\psi(r)|^2 r^2 dr$. The most probable position corresponds to the maximum of this probability distribution.

Solution:

The given wave function for the ground state of the hydrogen atom is:

$$\psi(r) = (\pi a_0^3)^{-1/2} \exp\left(\frac{-r}{a_0}\right)$$

The probability density in spherical coordinates is given by:

$$P(r) = |\psi(r)|^2 r^2$$

First, calculate $|\psi(r)|^2$:

$$|\psi(r)|^2 = (\pi a_0^3)^{-1} \exp\left(\frac{-2r}{a_0}\right)$$

The probability density becomes:

$$P(r) = (\pi a_0^3)^{-1} \exp\left(\frac{-2r}{a_0}\right) r^2$$

To find the most probable position, we need to maximize $P(r)$. This can be done by taking the derivative of $P(r)$ with respect to r and setting it to zero:

$$\frac{dP(r)}{dr} = 0$$

Let's compute the derivative:

$$\frac{dP(r)}{dr} = \frac{d}{dr} \left[(\pi a_0^3)^{-1} r^2 \exp\left(\frac{-2r}{a_0}\right) \right]$$

Using the product rule:

$$\frac{dP(r)}{dr} = (\pi a_0^3)^{-1} \left[\frac{d}{dr} (r^2) \exp\left(\frac{-2r}{a_0}\right) + r^2 \frac{d}{dr} \left(\exp\left(\frac{-2r}{a_0}\right) \right) \right]$$

First, compute the derivative of r^2 :

$$\frac{d}{dr}(r^2) = 2r$$

Next, compute the derivative of $\exp\left(\frac{-2r}{a_0}\right)$:

$$\frac{d}{dr}\left(\exp\left(\frac{-2r}{a_0}\right)\right) = \exp\left(\frac{-2r}{a_0}\right)\left(\frac{-2}{a_0}\right)$$

Substituting these results back into the expression for $\frac{dP(r)}{dr}$:

$$\frac{dP(r)}{dr} = (\pi a_0^3)^{-1} \left[2r \exp\left(\frac{-2r}{a_0}\right) + r^2 \exp\left(\frac{-2r}{a_0}\right)\left(\frac{-2}{a_0}\right) \right]$$

Factor out $\exp\left(\frac{-2r}{a_0}\right)$:

$$\frac{dP(r)}{dr} = (\pi a_0^3)^{-1} \exp\left(\frac{-2r}{a_0}\right) \left[2r - \frac{2r^2}{a_0} \right]$$

Set this expression equal to zero to find the maximum:

$$2r - \frac{2r^2}{a_0} = 0$$

Factor out $2r$:

$$2r \left(1 - \frac{r}{a_0} \right) = 0$$

This gives two solutions:

$$r = 0 \quad \text{or} \quad r = a_0$$

Since $r = 0$ corresponds to the nucleus where the probability is not maximum, the most probable position is $r = a_0$.

Conclusion:

The most probable position of the electron in the hydrogen atom's ground state is $r = a_0$, which corresponds to the radius of the first Bohr orbit. This result is consistent with the classical Bohr model of the atom, where the electron is most likely to be found at this radius.

53 Let $\vec{\sigma}$ be the vector operator with components equal to Pauli's spin matrices $\sigma_x, \sigma_y, \sigma_z$. If \vec{a} and \vec{b} are vectors in 3D space, prove the identity $(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\sigma} \cdot (\vec{a} \times \vec{b})$.

Introduction:

The Pauli matrices are often used in quantum mechanics to describe spin- $\frac{1}{2}$ particles. These matrices can be combined into a vector operator $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, where σ_x, σ_y , and σ_z are the Pauli matrices. The goal is to prove the given identity, which relates the product of two such operators to the dot product and cross product of the vectors \vec{a} and \vec{b} .

Solution:

The Pauli matrices are defined as:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Let $\vec{a} = (a_x, a_y, a_z)$ and $\vec{b} = (b_x, b_y, b_z)$. The dot products are:

$$\vec{\sigma} \cdot \vec{a} = a_x \sigma_x + a_y \sigma_y + a_z \sigma_z$$

$$\vec{\sigma} \cdot \vec{b} = b_x \sigma_x + b_y \sigma_y + b_z \sigma_z$$

We need to compute $(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b})$:

$$(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = (a_x \sigma_x + a_y \sigma_y + a_z \sigma_z)(b_x \sigma_x + b_y \sigma_y + b_z \sigma_z)$$

Expanding the product:

$$\begin{aligned} (\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) &= a_x b_x \sigma_x^2 + a_x b_y \sigma_x \sigma_y + a_x b_z \sigma_x \sigma_z \\ &\quad + a_y b_x \sigma_y \sigma_x + a_y b_y \sigma_y^2 + a_y b_z \sigma_y \sigma_z \\ &\quad + a_z b_x \sigma_z \sigma_x + a_z b_y \sigma_z \sigma_y + a_z b_z \sigma_z^2 \end{aligned}$$

Recall the following properties of the Pauli matrices:

$$\sigma_i \sigma_j = \delta_{ij} I + i\epsilon_{ijk} \sigma_k$$

where δ_{ij} is the Kronecker delta and ϵ_{ijk} is the Levi-Civita symbol.

Using these properties:

$$\begin{aligned} \sigma_x^2 &= \sigma_y^2 = \sigma_z^2 = I \\ \sigma_x \sigma_y &= i\sigma_z, \quad \sigma_y \sigma_x = -i\sigma_z \\ \sigma_y \sigma_z &= i\sigma_x, \quad \sigma_z \sigma_y = -i\sigma_x \\ \sigma_z \sigma_x &= i\sigma_y, \quad \sigma_x \sigma_z = -i\sigma_y \end{aligned}$$

Substituting these into the expanded expression:

$$(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = a_x b_x I + a_y b_y I + a_z b_z I + i(a_x b_y - a_y b_x) \sigma_z + i(a_y b_z - a_z b_y) \sigma_x + i(a_z b_x - a_x b_z) \sigma_y$$

This expression can be rewritten as:

$$(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = (\vec{a} \cdot \vec{b})I + i\vec{\sigma} \cdot (\vec{a} \times \vec{b})$$

Since I is the identity matrix, we can drop it:

$$(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\sigma} \cdot (\vec{a} \times \vec{b})$$

Conclusion:

The identity is proved, demonstrating that the product of two Pauli vector operators can be expressed as the sum of the dot product and an imaginary term involving the cross product. This result is significant in quantum mechanics, particularly in the study of spin interactions.

AP

54 The normalized wave function for the electron in the ground state of the hydrogen atom is given by $\psi(r) = \frac{1}{(\pi a_0^3)^{1/2}} e^{-r/a_0}$ where a_0 is the radius of the first Bohr orbit. Calculate $\langle r \rangle$ and $\langle \frac{1}{r} \rangle$.

Introduction:

The expectation values $\langle r \rangle$ and $\langle \frac{1}{r} \rangle$ describe the average radial distance and the average inverse radial distance of the electron, respectively. These expectation values are important for understanding the quantum mechanical properties of the hydrogen atom.

The expectation values can be calculated using the following integrals:

$$\langle r \rangle = \int_0^\infty r |\psi(r)|^2 r^2 dr$$

$$\langle \frac{1}{r} \rangle = \int_0^\infty \frac{1}{r} |\psi(r)|^2 r^2 dr$$

Solution:

The given normalized wave function is:

$$\psi(r) = \frac{1}{(\pi a_0^3)^{1/2}} e^{-r/a_0}$$

The corresponding probability density is:

$$|\psi(r)|^2 = \frac{1}{\pi a_0^3} e^{-2r/a_0}$$

1. Calculation of $\langle r \rangle$:

The expectation value is given by:

$$\langle r \rangle = \int_0^\infty r |\psi(r)|^2 r^2 dr$$

Substituting the probability density:

$$\langle r \rangle = \int_0^\infty r \cdot \frac{1}{\pi a_0^3} e^{-2r/a_0} r^2 dr$$

$$\langle r \rangle = \frac{1}{\pi a_0^3} \int_0^\infty r^3 e^{-2r/a_0} dr$$

Let's perform a substitution: let $u = \frac{2r}{a_0}$, so $du = \frac{2}{a_0} dr$, or equivalently, $dr = \frac{a_0}{2} du$. Also, $r = \frac{a_0 u}{2}$.

Substituting into the integral gives:

$$\langle r \rangle = \frac{1}{\pi a_0^3} \int_0^\infty \left(\frac{a_0 u}{2} \right)^3 \cdot \frac{a_0}{2} e^{-u} du$$

$$\langle r \rangle = \frac{a_0^4}{4\pi a_0^3} \int_0^\infty u^3 e^{-u} du$$

$$\langle r \rangle = \frac{a_0}{4\pi} \int_0^\infty u^3 e^{-u} du$$

The integral $\int_0^\infty u^3 e^{-u} du$ is a standard gamma function integral, $\Gamma(4) = 3! = 6$.

Thus:

$$\langle r \rangle = \frac{a_0}{4} \times 6 = \frac{3a_0}{2}$$

So, the expectation value $\langle r \rangle$ is:

$$\boxed{\langle r \rangle = \frac{3a_0}{2}}$$

2. Calculation of $\langle \frac{1}{r} \rangle$:

The expectation value is given by:

$$\left\langle \frac{1}{r} \right\rangle = \int_0^\infty \frac{1}{r} |\psi(r)|^2 r^2 dr$$

Substituting the probability density:

$$\left\langle \frac{1}{r} \right\rangle = \int_0^\infty \frac{1}{r} \cdot \frac{1}{\pi a_0^3} e^{-2r/a_0} r^2 dr$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{\pi a_0^3} \int_0^\infty r e^{-2r/a_0} dr$$

Using the same substitution as before: $u = \frac{2r}{a_0}$, $dr = \frac{a_0}{2} du$, and $r = \frac{a_0 u}{2}$:

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{\pi a_0^3} \int_0^\infty \frac{a_0 u}{2} \cdot \frac{a_0}{2} e^{-u} du$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{a_0^2}{\pi a_0^3} \int_0^\infty u e^{-u} du$$

The integral $\int_0^\infty u e^{-u} du$ is a standard gamma function integral, $\Gamma(2) = 1! = 1$.

Thus:

$$\left\langle \frac{1}{r} \right\rangle = \frac{a_0^2}{\pi a_0^3} \times 1 = \frac{1}{a_0}$$

So, the expectation value $\langle \frac{1}{r} \rangle$ is:

$$\boxed{\left\langle \frac{1}{r} \right\rangle = \frac{1}{a_0}}$$

Conclusion:

The calculated expectation values for the radial distance and its inverse are $\langle r \rangle = \frac{3a_0}{4}$ and $\langle \frac{1}{r} \rangle = \frac{1}{a_0}$. These results are consistent with the quantum mechanical description of the hydrogen atom.

AP

55 Using the definition $\vec{L} = \vec{r} \times \vec{p}$ of the orbital angular momentum operator, evaluate $[L_x, L_y]$.

Introduction:

The orbital angular momentum operator \vec{L} is defined as $\vec{L} = \vec{r} \times \vec{p}$, where \vec{r} is the position operator and \vec{p} is the momentum operator. The components of the angular momentum operator are given by:

$$L_x = yp_z - zp_y, \quad L_y = zp_x - xp_z, \quad \text{and} \quad L_z = xp_y - yp_x.$$

We want to evaluate the commutator $[L_x, L_y]$.

Solution:

Start with the definitions of L_x and L_y :

$$L_x = yp_z - zp_y, \quad L_y = zp_x - xp_z.$$

The commutator is:

$$[L_x, L_y] = [yp_z - zp_y, zp_x - xp_z].$$

Expanding the commutator using the distributive property:

$$[L_x, L_y] = [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z].$$

We will evaluate each of these commutators individually.

1. Evaluate $[yp_z, zp_x]$:

$$[yp_z, zp_x] = y[p_z, z]p_x + [y, z]p_zp_x.$$

Since $[y, z] = 0$ (different components commute), we are left with:

$$[yp_z, zp_x] = y[p_z, z]p_x.$$

The commutator $[p_z, z] = -i\hbar$, so:

$$[yp_z, zp_x] = -i\hbar yp_x.$$

2. Evaluate $[yp_z, xp_z]$:

$$[yp_z, xp_z] = [y, x]p_z^2 + y[p_z, x]p_z.$$

Again, $[y, x] = 0$ (different components commute), and $[p_z, x] = 0$, so:

$$[yp_z, xp_z] = 0.$$

3. Evaluate $[zp_y, zp_x]$:

$$[zp_y, zp_x] = z[p_y, z]p_x + [z, z]p_y p_x.$$

Since $[z, z] = 0$ and $[p_y, z] = 0$ (different components commute), we get:

$$[zp_y, zp_x] = 0.$$

4. Evaluate $[zp_y, xp_z]$:

$$[zp_y, xp_z] = [z, x]p_y p_z + z[p_y, x]p_z.$$

Since $[z, x] = 0$ and $[p_y, x] = i\hbar$, we have:

$$[zp_y, xp_z] = i\hbar zp_z.$$

Putting it all together:

$$[L_x, L_y] = -i\hbar yp_x + 0 + 0 + i\hbar zp_z.$$

This can be rewritten as:

$$[L_x, L_y] = i\hbar(zp_z - yp_x).$$

Notice that $zp_z - yp_x$ is the expression for L_z . Therefore:

$$[L_x, L_y] = i\hbar L_z.$$

Conclusion:

The commutator $[L_x, L_y]$ is given by:

$$\boxed{[L_x, L_y] = i\hbar L_z}.$$

This result is consistent with the standard commutation relations for the components of angular momentum in quantum mechanics.

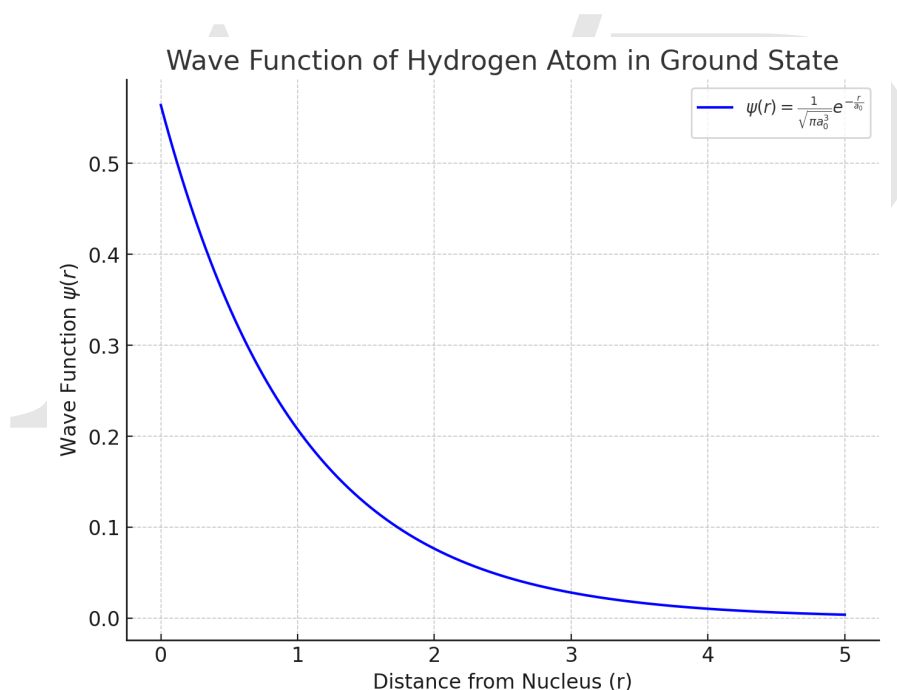
56 Calculate the probability of finding the electron within a distance r_0 of the proton in the ground state.

Introduction:

The normalized wave function for an electron in the ground state of the hydrogen atom is given by:

$$\psi(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}$$

where a_0 is the Bohr radius, representing the most probable distance between the electron and the nucleus in a hydrogen atom. The wave function $\psi(r)$ describes the quantum state of the electron in the hydrogen atom, and **its square gives the probability density of finding the electron at a distance r from the nucleus.** **Wave Function Graph:** The graph below illustrates the ground state wave function $\psi(r)$ as a function of distance r from the nucleus, showing an exponential decay from the nucleus.



Solution:

The probability of finding the electron within a distance r_0 from the proton is given by the integral of the probability density function over the desired range:

$$P(r \leq r_0) = \int_0^{r_0} |\psi(r)|^2 4\pi r^2 dr$$

Substitute the wave function $\psi(r)$:

$$P(r \leq r_0) = \int_0^{r_0} \left(\frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} \right)^2 4\pi r^2 dr$$

Simplifying, we get:

$$P(r \leq r_0) = \frac{4}{a_0^3} \int_0^{r_0} r^2 e^{-\frac{2r}{a_0}} dr$$

Now, evaluate the integral using the formula for the integral of $r^2 e^{-\alpha r}$:

$$\int_0^{r_0} r^2 e^{-\frac{2r}{a_0}} dr = \left(\frac{a_0^3}{8} \right) \left(1 - e^{-\frac{2r_0}{a_0}} \left(1 + \frac{2r_0}{a_0} + \frac{2r_0^2}{a_0^2} \right) \right)$$

Substitute this back to find the probability:

$$P(r \leq r_0) = 1 - e^{-\frac{2r_0}{a_0}} \left(1 + \frac{2r_0}{a_0} + \frac{2r_0^2}{a_0^2} \right)$$

Conclusion:

This probability distribution reflects the quantum mechanical nature of the electron in the hydrogen atom, where there is a high probability of finding the electron close to the nucleus, and **this probability decreases as the distance increases**. it helps predict atomic behavior and electron interactions.

57 If \hat{x} and \hat{p} are the position and momentum operators, prove the commutation relation $[\hat{p}^2, \hat{x}] = -2i\hbar\hat{p}$

Introduction:

In quantum mechanics, the position (\hat{x}) and momentum (\hat{p}) operators are fundamental operators that follow specific commutation relations. The commutation relation between these operators reflects the uncertainty principle, which states that the position and momentum of a particle cannot be precisely known simultaneously. One of the important commutation relations involving these operators is $[\hat{p}^2, \hat{x}] = -2i\hbar\hat{p}$.

Solution:

To prove the commutation relation $[\hat{p}^2, \hat{x}] = -2i\hbar\hat{p}$, we start by using the basic commutation relation between position and momentum operators:

$$[\hat{x}, \hat{p}] = i\hbar$$

1. Consider the expression for the commutator $[\hat{p}^2, \hat{x}]$:

$$[\hat{p}^2, \hat{x}] = \hat{p}[\hat{p}, \hat{x}] + [\hat{p}, \hat{x}]\hat{p}$$

2. Substitute the known commutation relation $[\hat{x}, \hat{p}] = i\hbar$, which gives:

$$[\hat{p}, \hat{x}] = -i\hbar$$

Therefore,

$$[\hat{p}^2, \hat{x}] = \hat{p}(-i\hbar) + (-i\hbar)\hat{p}$$

$$[\hat{p}^2, \hat{x}] = -i\hbar\hat{p} - i\hbar\hat{p}$$

$$[\hat{p}^2, \hat{x}] = -2i\hbar\hat{p}$$

Conclusion:

The commutation relation $[\hat{p}^2, \hat{x}] = -2i\hbar\hat{p}$ demonstrates how the momentum operator squared interacts with the position operator in quantum mechanics. This relation highlights the non-commutative nature of quantum operators, which is a key aspect of the uncertainty principle.

58 Write down Pauli spin matrices. Express J_x , J_y , and J_z in terms of Pauli spin matrices.

Introduction:

The Pauli spin matrices are a set of three 2×2 complex matrices that represent the spin operators for a spin- $\frac{1}{2}$ particle in quantum mechanics. They are fundamental in describing the spin properties of particles such as electrons. The Pauli matrices are usually denoted by σ_x , σ_y , and σ_z .

Solution:

The Pauli spin matrices are defined as:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The spin angular momentum operators J_x , J_y , and J_z for a spin- $\frac{1}{2}$ particle can be expressed in terms of the Pauli matrices as follows:

$$J_x = \frac{\hbar}{2}\sigma_x, \quad J_y = \frac{\hbar}{2}\sigma_y, \quad J_z = \frac{\hbar}{2}\sigma_z$$

Conclusion:

The Pauli spin matrices σ_x , σ_y , and σ_z form the basis for representing the spin operators J_x , J_y , and J_z of a spin- $\frac{1}{2}$ particle. These matrices are used extensively in quantum mechanics to describe the spin state of particles, calculate spin dynamics, and solve various quantum systems involving spin. Their importance lies in their ability to represent the intrinsic angular momentum properties of fundamental particles.

59 Using the commutation relations $[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$, deduce the commutation relation between the components of angular momentum operator \mathbf{L} .

Introduction:

In quantum mechanics, the angular momentum operator \mathbf{L} has three components: L_x , L_y , and L_z . These components satisfy certain commutation relations derived from the fundamental commutation relations between position (x, y, z) and momentum (p_x, p_y, p_z) operators. The goal is to deduce the commutation relations among L_x , L_y , and L_z .

Solution:

The angular momentum operators in quantum mechanics are defined as:

$$L_x = yp_z - zp_y, \quad L_y = zp_x - xp_z, \quad L_z = xp_y - yp_x$$

We use the commutation relations between position and momentum operators:

$$[x, p_x] = i\hbar, \quad [y, p_y] = i\hbar, \quad [z, p_z] = i\hbar$$

and all other commutators like $[x, p_y]$, $[x, p_z]$, etc., are zero.

Now, let us compute the commutation relations between the components of \mathbf{L} .

1. Commutator of L_x and L_y :

$$[L_x, L_y] = [(yp_z - zp_y), (zp_x - xp_z)]$$

Expanding the commutator:

$$[L_x, L_y] = yp_z zp_x - yp_z xp_z - zp_y zp_x + zp_y xp_z$$

Using the commutation relations:

$$[L_x, L_y] = y[p_z, z]p_x + [z, p_z]p_y x = i\hbar L_z$$

2. Commutator of L_y and L_z :

$$[L_y, L_z] = [(zp_x - xp_z), (xp_y - yp_x)]$$

Expanding the commutator:

$$[L_y, L_z] = zp_x xp_y - zp_x yp_x - xp_z xp_y + xp_z yp_x$$

Using the commutation relations:

$$[L_y, L_z] = z[p_x, x]p_y + [x, p_x]p_z y = i\hbar L_x$$

3. Commutator of L_z and L_x :

$$[L_z, L_x] = [(xp_y - yp_x), (yp_z - zp_y)]$$

Expanding the commutator:

$$[L_z, L_x] = xp_y yp_z - xp_y zp_y - yp_x yp_z + yp_x zp_y$$

Using the commutation relations:

$$[L_z, L_x] = x[p_y, y]p_z + [y, p_y]p_x z = i\hbar L_y$$

Conclusion:

We have deduced the commutation relations between the components of the angular momentum operator \mathbf{L} :

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y$$

These relations reflect the underlying algebraic structure of angular momentum in quantum mechanics, which is fundamental to the study of rotational symmetries and quantum states.

60 Solve the Schrödinger equation for a particle in a three-dimensional rectangular potential barrier. Explain the terms degenerate and non-degenerate states in this context.

Introduction:

The Schrödinger equation is a fundamental equation in quantum mechanics that describes how the quantum state of a physical system changes with time. For a particle in a three-dimensional rectangular potential barrier, we solve the time-independent Schrödinger equation, which is given by:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x, y, z) + V(x, y, z)\psi(x, y, z) = E\psi(x, y, z), \quad (1)$$

where:

- \hbar is the reduced Planck's constant,
- m is the mass of the particle,
- $\psi(x, y, z)$ is the wave function,
- $V(x, y, z)$ is the potential energy,
- E is the total energy of the particle.

In a three-dimensional rectangular potential barrier, the potential $V(x, y, z)$ is defined as:

$$V(x, y, z) = \begin{cases} 0 & \text{if } 0 < x < a, 0 < y < b, 0 < z < c, \\ V_0 & \text{otherwise,} \end{cases}$$

where a , b , and c are the dimensions of the potential well.

Graph of the Wave Function:

To visualize the behavior of the wave function $\psi(x, y, z)$ inside the potential barrier, a plot is generated below to illustrate its variation in two dimensions:

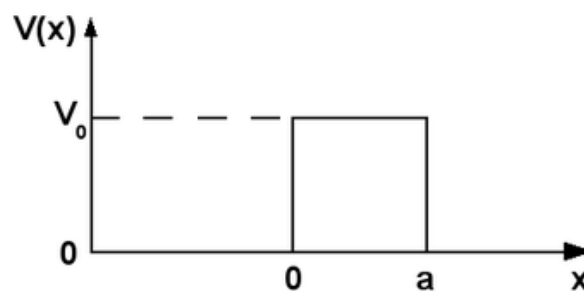


Figure 1: Wave Function for a Particle in a Rectangular Potential Barrier

Solution:

To solve the Schrödinger equation, we employ the method of separation of variables. Assume the wave function can be separated into three parts:

$$\psi(x, y, z) = X(x)Y(y)Z(z). \quad (2)$$

Substitute this into the Schrödinger equation:

$$-\frac{\hbar^2}{2m} \left(\frac{d^2 X}{dx^2} YZ + X \frac{d^2 Y}{dy^2} Z + XY \frac{d^2 Z}{dz^2} \right) + V(x, y, z)XYZ = EXYZ. \quad (3)$$

Dividing through by XYZ , we get:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{X} \frac{d^2 X}{dx^2} + \frac{1}{Y} \frac{d^2 Y}{dy^2} + \frac{1}{Z} \frac{d^2 Z}{dz^2} \right) + V(x, y, z) = E. \quad (4)$$

Since the potential $V(x, y, z)$ is zero inside the barrier, we can separate the equation into three independent differential equations:

$$\frac{d^2 X}{dx^2} = -k_x^2 X(x), \quad \frac{d^2 Y}{dy^2} = -k_y^2 Y(y), \quad \frac{d^2 Z}{dz^2} = -k_z^2 Z(z), \quad (5)$$

where $k_x^2 = \frac{2mE_x}{\hbar^2}$, $k_y^2 = \frac{2mE_y}{\hbar^2}$, and $k_z^2 = \frac{2mE_z}{\hbar^2}$ are the separation constants, and $E = E_x + E_y + E_z$.

The general solutions for these equations inside the well are:

$$\begin{aligned} X(x) &= A \sin(k_x x) + B \cos(k_x x), \\ Y(y) &= C \sin(k_y y) + D \cos(k_y y), \\ Z(z) &= E \sin(k_z z) + F \cos(k_z z). \end{aligned}$$

Applying boundary conditions $X(0) = X(a) = 0$, $Y(0) = Y(b) = 0$, and $Z(0) = Z(c) = 0$, the solutions reduce to:

$$\begin{aligned} X(x) &= A \sin\left(\frac{n_x \pi x}{a}\right), \quad n_x = 1, 2, 3, \dots, \\ Y(y) &= C \sin\left(\frac{n_y \pi y}{b}\right), \quad n_y = 1, 2, 3, \dots, \\ Z(z) &= E \sin\left(\frac{n_z \pi z}{c}\right), \quad n_z = 1, 2, 3, \dots \end{aligned}$$

The energy levels are given by:

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right). \quad (6)$$

Degenerate and Non-Degenerate States:

In the context of quantum mechanics, *degenerate states* refer to different quantum states that have the same energy. For the three-dimensional rectangular potential barrier, if multiple sets of quantum numbers (n_x, n_y, n_z) result in the same energy E_{n_x, n_y, n_z} , these states are degenerate.

A *non-degenerate state* is a quantum state that has a unique set of quantum numbers for a given energy level, meaning no other state shares the same energy.

For example, if $a = b = c$, then E_{n_x, n_y, n_z} depends only on the sum $n_x^2 + n_y^2 + n_z^2$. Thus, different combinations such as $(1, 1, 2)$ and $(2, 1, 1)$ will give the same energy, resulting in degeneracy. In contrast, if $a \neq b \neq c$, the energies are likely to be non-degenerate.

Conclusion:

The Schrödinger equation for a particle in a three-dimensional rectangular potential barrier shows that the energy levels depend on the dimensions of the barrier and the quantum numbers (n_x, n_y, n_z) . Degenerate states occur when different quantum states have the same energy, **which is influenced by the symmetry of the potential barrier**. Non-degenerate states occur when each state has a unique energy level. This concept is critical in understanding the behavior of quantum particles in confined geometries and has applications in **quantum wells, quantum dots, and nanotechnology**.