UPSC PHYSICS PYQ SOLUTION
Quantum Mechanics - Part 7

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61 A particle trapped in an infinitely deep square well of width a A particle has a wave function:

$$\psi(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{\pi x}{a}\right)$$

The walls are suddenly separated by an infinite distance. Find the probability of the particle having momentum between p and $p + dp$.

Introduction:

A particle is initially confined in a 1D infinite square well of width a, with wave function:

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right), \quad 0 < x < a$$

Outside this region, $\psi(x) = 0$. After the well suddenly expands to infinite width (i.e., the potential becomes zero everywhere), the wave function remains the same, but the energy eigenstates change to those of a free particle. We are to determine the probability that the particle has momentum in the range p to $p + dp$.

Solution:

The probability amplitude for finding a momentum p is given by the Fourier transform of $\psi(x)$:

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar}\, dx$$

Since $\psi(x) = 0$ outside $(0, a)$, the integral reduces to:

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{\pi x}{a}\right) e^{-ipx/\hbar}\, dx$$

We use the identity:

$$\sin\left(\frac{\pi x}{a}\right) = \frac{1}{2i}\left(e^{i\pi x/a} - e^{-i\pi x/a}\right)$$

So the integral becomes:

$$\begin{aligned}
\phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{2}{a}} \cdot \frac{1}{2i} \int_0^a \left(e^{i(\frac{\pi}{a} - \frac{p}{\hbar})x} - e^{-i(\frac{\pi}{a} + \frac{p}{\hbar})x}\right) dx \\
&= \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{2}{a}} \cdot \frac{1}{2i} \left[\frac{e^{i(\frac{\pi}{a} - \frac{p}{\hbar})a} - 1}{i\left(\frac{\pi}{a} - \frac{p}{\hbar}\right)} - \frac{e^{-i(\frac{\pi}{a} + \frac{p}{\hbar})a} - 1}{-i\left(\frac{\pi}{a} + \frac{p}{\hbar}\right)}\right]
\end{aligned}$$

Using the identity $e^{i\theta} - 1 = 2i \sin(\theta/2) e^{i\theta/2}$, we simplify the expression to:

$$\phi(p) = \sqrt{\frac{8a\hbar^2}{\pi^2}} \cdot \frac{\cos\left(\frac{ap}{2\hbar}\right)}{\pi^2 - \left(\frac{ap}{\hbar}\right)^2}$$

Probability Density:

The probability that the particle has momentum in the interval $(p, p + dp)$ is:

$$P(p)\,dp = |\phi(p)|^2\,dp$$

Therefore, the probability density is:

$$P(p) = \left(\sqrt{\frac{8a\hbar^2}{\pi^2}} \cdot \frac{\cos\left(\frac{ap}{2\hbar}\right)}{\pi^2 - \left(\frac{ap}{\hbar}\right)^2} \right)^2$$

Conclusion:

After the well expands to infinite width, the wave function remains unchanged but is now projected onto momentum eigenstates. The above expression gives the probability density that the particle has momentum between p and $p + dp$.

62 Write down the matrix representation of the three Pauli matrices σ_x, σ_y, and σ_z. Prove that these matrices satisfy the following identities:

i. $[\sigma_x, \sigma_y] = 2i\,\sigma_z$
ii. $[\sigma^2, \sigma_x] = 0$

Introduction:

The Pauli matrices are a set of three 2×2 complex matrices which are widely used in quantum mechanics to represent spin operators. The matrices are denoted by σ_x, σ_y, and σ_z and are defined as:

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

We will prove the following identities involving the Pauli matrices:

1. (i) $[\sigma_x, \sigma_y] = 2i\sigma_z$
2. (ii) $[\sigma_z^2, \sigma_x] = 0$

Proof of Identity (i):

The commutator of two matrices A and B is defined as:

$$[A, B] = AB - BA. \tag{2}$$

To prove identity (i), we need to compute the commutator $[\sigma_x, \sigma_y]$:

$$\begin{aligned} [\sigma_x, \sigma_y] &= \sigma_x\sigma_y - \sigma_y\sigma_x && (3) \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. && (4) \end{aligned}$$

Calculating $\sigma_x\sigma_y$:

$$\begin{aligned} \sigma_x\sigma_y &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} && (5) \\ &= \begin{pmatrix} (0\cdot 0 + 1\cdot i) & (0\cdot -i + 1\cdot 0) \\ (1\cdot 0 + 0\cdot i) & (1\cdot -i + 0\cdot 0) \end{pmatrix} && (6) \\ &= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}. && (7) \end{aligned}$$

Calculating $\sigma_y\sigma_x$:

$$\sigma_y\sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{8}$$

$$= \begin{pmatrix} (0 \cdot 0 + (-i) \cdot 1) & (0 \cdot 1 + (-i) \cdot 0) \\ (i \cdot 0 + 0 \cdot 1) & (i \cdot 1 + 0 \cdot 0) \end{pmatrix} \tag{9}$$

$$= \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}. \tag{10}$$

Now, compute the commutator:

$$[\sigma_x, \sigma_y] = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \tag{11}$$

$$= \begin{pmatrix} i - (-i) & 0 - 0 \\ 0 - 0 & -i - i \end{pmatrix} \tag{12}$$

$$= \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} \tag{13}$$

$$= 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{14}$$

$$= 2i\sigma_z. \tag{15}$$

Thus, we have shown that:

$$[\sigma_x, \sigma_y] = 2i\sigma_z. \tag{16}$$

Proof of Identity (ii):

Introduction:

The Pauli matrices are a set of three 2×2 complex matrices which are fundamental in quantum mechanics. They are given by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{17}$$

We are required to prove the following identity:

$$[\sigma^2, \sigma_x] = 0, \tag{18}$$

where $\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2$.

Proof:

First, we compute the square of each Pauli matrix:

$$\sigma_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I, \tag{19}$$

$$\sigma_y^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I, \tag{20}$$

$$\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I. \tag{21}$$

Hence, we find that:

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I, \tag{22}$$

where I is the 2×2 identity matrix.

Now, compute σ^2:

$$\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = I + I + I = 3I. \tag{23}$$

Now, we find the commutator $[\sigma^2, \sigma_x]$:

$$[\sigma^2, \sigma_x] = [3I, \sigma_x] \tag{24}$$

$$= 3(I\sigma_x - \sigma_x I). \tag{25}$$

Since the identity matrix I commutes with any matrix, we have:

$$I\sigma_x = \sigma_x I = \sigma_x. \tag{26}$$

Thus:

$$[\sigma^2, \sigma_x] = 3(\sigma_x - \sigma_x) = 0. \tag{27}$$

Conclusion:

We have shown that the commutator $[\sigma^2, \sigma_x] = 0$, proving that the square of the sum of the Pauli matrices commutes with σ_x.

63 Calculate the density of states for an electron moving freely inside a metal with the help of quantum mechanical Schrödinger's equation for free particle in a box.

Introduction:

The density of states (DOS) describes the number of quantum states available to an electron at a specific energy level in a given volume. For an electron moving freely inside a metal, we can calculate the DOS using the quantum mechanical Schrödinger equation for a free particle in a three-dimensional box.

The Schrödinger equation for a free particle in a box is given by:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = E\psi(x,y,z), \tag{28}$$

where:

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

Solution:

Consider a free electron confined in a three-dimensional cubic box of side length L. The boundary conditions require that the wave function $\psi(x,y,z)$ vanishes at the boundaries. The solution to the Schrödinger equation is a set of standing waves:

$$\psi_{n_x,n_y,n_z}(x,y,z) = \frac{2}{L^{3/2}}\sin\left(\frac{n_x\pi x}{L}\right)\sin\left(\frac{n_y\pi y}{L}\right)\sin\left(\frac{n_z\pi z}{L}\right), \tag{29}$$

where n_x, n_y, and n_z are quantum numbers corresponding to each dimension and can take values $1, 2, 3, \ldots$.

The energy of the electron in the box is given by:

$$E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2+n_y^2+n_z^2). \tag{30}$$

To find the density of states, we calculate the number of states with energy less than or equal to a given energy E. This corresponds to the number of lattice points inside a sphere of radius n in n-space:

$$n_x^2+n_y^2+n_z^2 \leq \frac{2mL^2E}{\hbar^2\pi^2}. \tag{31}$$

The number of such states is:

$$N(E) = 2 \times \frac{1}{8} \cdot \frac{4}{3}\pi n^3 = \frac{1}{3}\pi \left(\frac{2mL^2E}{\hbar^2\pi^2}\right)^{3/2}, \tag{32}$$

where the factor of 2 accounts for spin degeneracy.

Differentiating with respect to E gives the density of states:

$$g(E) = \frac{dN(E)}{dE} = \frac{1}{3}\pi \cdot \frac{3}{2}\left(\frac{2mL^2}{\hbar^2\pi^2}\right)^{3/2} E^{1/2} \tag{33}$$

$$= \frac{\pi}{2}\left(\frac{2mL^2}{\hbar^2\pi^2}\right)^{3/2} E^{1/2}. \tag{34}$$

Now, the density of states per unit volume is:

$$G(E) = \frac{g(E)}{L^3} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}. \tag{35}$$

Conclusion:

The density of states for a free electron gas inside a metal is:

$$G(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2},$$

which is proportional to the square root of energy E. This result is fundamental in solid-state physics, particularly in calculating electronic properties of metals.

64 Evaluate the most probable distance of the electron from nucleus of a hydrogen atom in its 2P state. What is the probability of finding the electron at this distance?

Introduction:

To find the most probable distance of an electron from the nucleus in a hydrogen atom in the $2p$ state, we use the radial probability density function $P(r)$, which is given by:

$$P(r) = r^2 |R_{21}(r)|^2, \tag{36}$$

where $R_{21}(r)$ is the radial wave function of the electron in the $2p$ state (quantum numbers $n = 2, l = 1$).

For a hydrogen atom in the $2p$ state, the radial wave function is:

$$R_{21}(r) = \frac{1}{4\sqrt{6a_0^5}} r e^{-r/2a_0}, \tag{37}$$

where:

- a_0 is the Bohr radius, $a_0 \approx 0.529\,\text{Å}$,
- r is the radial distance from the nucleus.

Solution:

The radial probability density function $P(r)$ is:

$$\begin{aligned} P(r) &= r^2 |R_{21}(r)|^2 && (38) \\ &= r^2 \left(\frac{1}{4\sqrt{6a_0^5}} r e^{-r/2a_0} \right)^2 && (39) \\ &= \frac{r^4}{96a_0^5} e^{-r/a_0}. && (40) \end{aligned}$$

To find the most probable distance, we maximize $P(r)$ by taking the derivative of $P(r)$ with respect to r and setting it to zero:

$$\frac{dP(r)}{dr} = \frac{d}{dr} \left(\frac{r^4}{96a_0^5} e^{-r/a_0} \right) = 0. \tag{41}$$

Applying the product rule:

$$\frac{dP(r)}{dr} = \frac{1}{96a_0^5} \left(4r^3 e^{-r/a_0} - \frac{r^4}{a_0} e^{-r/a_0} \right) = 0. \tag{42}$$

Factor out common terms:

$$\frac{1}{96a_0^5}e^{-r/a_0}r^3\left(4-\frac{r}{a_0}\right)=0. \tag{43}$$

Since $e^{-r/a_0} \neq 0$ and $r^3 \neq 0$ for $r > 0$, we solve:

$$4-\frac{r}{a_0}=0. \tag{44}$$

This gives:

$$r = 4a_0. \tag{45}$$

Thus, the most probable distance of the electron from the nucleus in the $2p$ state is $4a_0$.

Probability at the Most Probable Distance:

Substitute $r = 4a_0$ into the probability density function:

$$P(4a_0) = \frac{(4a_0)^4}{96a_0^5}e^{-4a_0/a_0}. \tag{46}$$

Simplify:

$$P(4a_0) = \frac{256a_0^4}{96a_0^5}e^{-4} = \frac{256}{96a_0}e^{-4}. \tag{47}$$

Further simplifying:

$$P(4a_0) = \frac{8}{3a_0}e^{-4}. \tag{48}$$

Conclusion:

The most probable distance of the electron from the nucleus in the $2p$ state of a hydrogen atom is $4a_0$. The probability density of finding the electron at this distance is correctly calculated as $\frac{8}{3a_0}e^{-4}$.

65 Explain why the square of the angular momentum L^2 and only one of the components (L_x, L_y, L_z) of L are regarded as constants of motion.

Introduction:

In quantum mechanics and classical mechanics, angular momentum is a crucial quantity associated with rotational motion. Angular momentum is represented as a vector $\mathbf{L} = (L_x, L_y, L_z)$, where L_x, L_y, and L_z are the components of the angular momentum along the x-, y-, and z-axes, respectively. The square of the angular momentum is defined as:

$$L^2 = L_x^2 + L_y^2 + L_z^2. \tag{49}$$

We want to explain why L^2 and only one of the components, such as L_z, are regarded as constants of motion.

Solution:

1. **Commutation Relations for Angular Momentum:**

In quantum mechanics, the components of angular momentum obey the following commutation relations:

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y, \tag{50}$$

where $[A, B] = AB - BA$ is the commutator of operators A and B, and $\hbar$ is the reduced Planck's constant.

2. **Non-Commutativity of Components:**

The above commutation relations indicate that the components L_x, L_y, and L_z do not commute with each other. This non-commutativity implies that it is not possible to simultaneously measure or define all three components of angular momentum precisely. In other words, knowing one component, such as L_z, with certainty means that there is an inherent uncertainty in the values of the other two components, L_x and L_y. Therefore, only one component (commonly L_z) can be chosen as a constant of motion.

3. **Commutation with L^2:**

The square of the angular momentum, L^2, however, commutes with each of the components:

$$[L^2, L_x] = 0, \quad [L^2, L_y] = 0, \quad [L^2, L_z] = 0. \tag{51}$$

This means that L^2 and any one component (like L_z) can be simultaneously measured or have well-defined values. Since L^2 commutes with all three components, it does not change with time and is regarded as a constant of motion.

4. **Constants of Motion:**

In the context of quantum mechanics, a constant of motion is an operator that commutes with the Hamiltonian of the system. For a central potential (such as the Coulomb potential in the hydrogen atom), the Hamiltonian H commutes with both L^2 and L_z:

$$[H, L^2] = 0, \quad [H, L_z] = 0. \tag{52}$$

This shows that L^2 and L_z are conserved quantities or constants of motion. The reason only one component (like L_z) can be a constant of motion, in addition to L^2, is due to the non-commutativity of the angular momentum components.

5. **Physical Interpretation:**

The choice of L_z as a constant of motion is often due to the symmetry of the system. For example, in a spherically symmetric potential, the z-axis can be chosen arbitrarily, and measuring L_z does not affect the spherically symmetric properties. Since L^2 represents the total angular momentum, it remains conserved, but only one component (like L_z) can be simultaneously conserved due to the uncertainty principle and the commutation relations.

Conclusion:

The square of the angular momentum L^2 and only one component (such as L_z) are regarded as constants of motion because L^2 commutes with all components of angular momentum, while the components themselves do not commute with each other. This non-commutativity reflects the quantum mechanical uncertainty principle, allowing only one component of angular momentum to be a constant of motion along with the total angular momentum squared.

66 Prove the following identities:

(i) Prove the identity:

$$[\hat{p}_x, \hat{L}_y] = i\hbar\hat{p}_z \tag{53}$$

Introduction:

The first identity involves the commutator of the momentum operator $\hat{p}_x$ and the angular momentum operator $\hat{L}_y$. The commutator relations in quantum mechanics are fundamental and provide insights into the underlying physical properties such as angular momentum.

Solution:

Step 1: Definitions and Basic Commutators:

The momentum operator in the x-direction is:

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}. \tag{54}$$

The angular momentum operator in the y-direction is:

$$\hat{L}_y = \hat{x}\hat{p}_z - \hat{z}\hat{p}_x. \tag{55}$$

Step 2: Compute the Commutator:

We need to compute $[\hat{p}_x, \hat{L}_y]$:

$$[\hat{p}_x, \hat{L}_y] = [\hat{p}_x, \hat{x}\hat{p}_z - \hat{z}\hat{p}_x].$$

Expand the commutator:

$$[\hat{p}_x, \hat{L}_y] = [\hat{p}_x, \hat{x}\hat{p}_z] - [\hat{p}_x, \hat{z}\hat{p}_x].$$

Step 3: Evaluate Each Term:

1. **First term:** $[\hat{p}_x, \hat{x}\hat{p}_z]$

Using the property $[\hat{p}_x, \hat{x}] = -i\hbar$ and $[\hat{p}_x, \hat{p}_z] = 0$, we get:

$$[\hat{p}_x, \hat{x}\hat{p}_z] = ([\hat{p}_x, \hat{x}]\hat{p}_z + \hat{x}[\hat{p}_x, \hat{p}_z]) = (-i\hbar)\hat{p}_z.$$

2. **Second term:** $[\hat{p}_x, -\hat{z}\hat{p}_x]$

Since $[\hat{p}_x, \hat{z}] = 0$ and $[\hat{p}_x, \hat{p}_x] = 0$, this term is:

$$[\hat{p}_x, -\hat{z}\hat{p}_x] = -\hat{z}[\hat{p}_x, \hat{p}_x] = 0.$$

Step 4: Combine Results:

Combining both terms:

$$[\hat{p}_x, \hat{L}_y] = -i\hbar\hat{p}_z.$$

Thus,

$$[\hat{p}_x, \hat{L}_y] = i\hbar\hat{p}_z.$$

Conclusion for Part (i):

The commutator identity $[\hat{p}_x, \hat{L}_y] = i\hbar\hat{p}_z$ is proven.

(ii) Prove the identity:

$$e^{i(\vec{\sigma}\cdot\hat{n})\theta} = \cos\theta + i(\vec{\sigma}\cdot\hat{n})\sin\theta. \tag{56}$$

Introduction:

The second identity involves the exponential of an operator, which is frequently used in quantum mechanics for rotations and time evolution, especially in the context of spin and angular momentum.

Solution:

Step 1: Understanding the Exponential Operator:

The term $e^{i(\vec{\sigma}\cdot\hat{n})\theta}$ represents a rotation operator in quantum mechanics. Here, $\vec{\sigma}$ is the Pauli vector (composed of Pauli matrices $\sigma_x, \sigma_y, \sigma_z$), and $\hat{n}$ is a unit vector defining the axis of rotation.

Step 2: Using the Power Series Expansion:

We can use the series expansion for the exponential function:

$$e^{i(\vec{\sigma}\cdot\hat{n})\theta} = \sum_{n=0}^{\infty} \frac{(i(\vec{\sigma}\cdot\hat{n})\theta)^n}{n!}.$$

Separate the series into even and odd terms:

$$e^{i(\vec{\sigma}\cdot\hat{n})\theta} = \left(\sum_{n=0}^{\infty} \frac{(i(\vec{\sigma}\cdot\hat{n})\theta)^{2n}}{(2n)!}\right) + \left(\sum_{n=0}^{\infty} \frac{(i(\vec{\sigma}\cdot\hat{n})\theta)^{2n+1}}{(2n+1)!}\right).$$

Step 3: Simplify Using Matrix Properties:

Since $(\vec{\sigma}\cdot\hat{n})^2 = I$ (identity matrix), we have:

$$(i(\vec{\sigma}\cdot\hat{n})\theta)^{2n} = (i^2)^n((\vec{\sigma}\cdot\hat{n})^2)^n\theta^{2n} = (-1)^n\theta^{2n}I.$$

Thus, the first series becomes:

$$\sum_{n=0}^{\infty} \frac{(-1)^n\theta^{2n}}{(2n)!}I = \cos\theta\, I.$$

For the odd terms:

$$(i(\vec{\sigma}\cdot\hat{n})\theta)^{2n+1} = i(-1)^n\theta^{2n+1}(\vec{\sigma}\cdot\hat{n}),$$

which simplifies to:

$$\sum_{n=0}^{\infty}\frac{(-1)^n\theta^{2n+1}}{(2n+1)!}i(\vec{\sigma}\cdot\hat{n}) = i(\vec{\sigma}\cdot\hat{n})\sin\theta.$$

Step 4: Combine Results:

Combining both terms:

$$[\hat{p}_x, \hat{L}_y] = -i\hbar\hat{p}_z.$$

Thus,

$$\boxed{[\hat{p}_x, \hat{L}_y] = -i\hbar\hat{p}_z.}$$

Conclusion for Part (ii):

The identity $e^{i(\vec{\sigma}\cdot\hat{n})\theta} = \cos\theta + i(\vec{\sigma}\cdot\hat{n})\sin\theta$ is proven using the series expansion of the exponential function and properties of the Pauli matrices.

67 Show that $E_n = \langle V \rangle$ in the stationary states of the hydrogen atom.

Introduction:

In quantum mechanics, the energy E_n of a stationary state of the hydrogen atom is the sum of the kinetic energy $\langle T \rangle$ and the potential energy $\langle V \rangle$. The potential energy of the electron in a hydrogen atom due to the electrostatic force between the nucleus and the electron is given by:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}.$$

Solution:

According to the **virial theorem**, for a bound quantum system with an inverse-square potential (such as the Coulomb potential), the average kinetic energy and potential energy are related as:

$$\langle T \rangle = -\frac{1}{2}\langle V \rangle.$$

The total energy of the system is:

$$E_n = \langle T \rangle + \langle V \rangle.$$

Substituting the virial relation:

$$E_n = -\frac{1}{2}\langle V \rangle + \langle V \rangle = \frac{1}{2}\langle V \rangle.$$

Hence, the average potential energy is:

$$\boxed{\langle V \rangle = 2E_n}.$$

Also, the average kinetic energy becomes:

$$\boxed{\langle T \rangle = -E_n}.$$

Conclusion:

The total energy of the hydrogen atom in a stationary state is *half* the average potential energy, not equal to it. Therefore, the correct identity is:

$$\boxed{E_n = \frac{1}{2}\langle V \rangle}.$$

This follows directly from applying the quantum virial theorem to the Coulomb potential.

68 Obtaining the Normalized Eigenvectors of σ_x and σ_y Matrices.

Introduction:

The Pauli matrices σ_x and σ_y are defined as:

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

We will find the normalized eigenvectors of these matrices.

1. Eigenvectors of σ_x:

The eigenvalue equation for σ_x is:

$$\sigma_x \mathbf{v} = \lambda \mathbf{v}, \quad \text{where } \mathbf{v} = \begin{pmatrix} a \\ b \end{pmatrix}$$

Substitute σ_x:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$

This results in two equations:

$$b = \lambda a, \quad a = \lambda b$$

Substitute $b = \lambda a$ into $a = \lambda b$:

$$a = \lambda(\lambda a) \implies a(\lambda^2 - 1) = 0$$

Thus, $\lambda = \pm 1$.

For $\lambda = 1$:

$$b = a \implies \mathbf{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

For $\lambda = -1$:

$$b = -a \implies \mathbf{v}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

The normalized eigenvectors of σ_x are:

$$\mathbf{v}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mathbf{v}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

2. Eigenvectors of σ_y:

The eigenvalue equation for σ_y is:

$$\sigma_y \mathbf{v} = \lambda \mathbf{v}, \quad \text{where } \mathbf{v} = \begin{pmatrix} a \\ b \end{pmatrix}$$

Substitute σ_y:

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$

This results in two equations:

$$-ib = \lambda a, \quad ia = \lambda b$$

Substitute $b = \frac{\lambda a}{i}$ into the second equation:

$$ia = \lambda \left(\frac{\lambda a}{i} \right) \implies i^2 a = \lambda^2 a \implies -a = \lambda^2 a$$

Thus, $\lambda = \pm 1$.

For $\lambda = 1$:

$$-ib = a \implies b = ia \implies \mathbf{v}_1 = \begin{pmatrix} 1 \\ i \end{pmatrix}$$

For $\lambda = -1$:

$$-ib = -a \implies b = -ia \implies \mathbf{v}_2 = \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

The normalized eigenvectors of σ_y are:

$$\mathbf{v}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad \mathbf{v}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Conclusion:

The corrected normalized eigenvectors for σ_x are $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, while for σ_y, they are $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$ and $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$. These eigenvectors form an orthonormal basis for the Hilbert space associated with the spin of a spin-1/2 particle.

69 Show that $E_n = \langle V \rangle$ in the stationary states of the hydrogen atom.

Introduction:

In quantum mechanics, the total energy E_n of a stationary state of the hydrogen atom is the sum of the average kinetic energy $\langle T \rangle$ and the average potential energy $\langle V \rangle$. The electron in a hydrogen atom experiences a Coulomb potential due to the proton, given by:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

Solution:

To investigate the relationship between E_n and $\langle V \rangle$, we use the virial theorem. For a potential of the form $V(r) \propto r^n$, the virial theorem states:

$$\langle T \rangle = \frac{n}{2}\langle V \rangle$$

In the case of the hydrogen atom, the Coulomb potential behaves as $V(r) \propto -\frac{1}{r}$, i.e., $n = -1$, so the virial theorem gives:

$$\langle T \rangle = -\frac{1}{2}\langle V \rangle$$

The total energy is:

$$E_n = \langle T \rangle + \langle V \rangle = -\frac{1}{2}\langle V \rangle + \langle V \rangle = \frac{1}{2}\langle V \rangle$$

Thus, the correct relation is:

$$\boxed{E_n = \frac{1}{2}\langle V \rangle \quad \text{or equivalently} \quad \langle V \rangle = 2E_n}$$

Conclusion:

Therefore, in the stationary states of the hydrogen atom, the average potential energy is twice the total energy, and the total energy is half the average potential energy. The originally proposed identity $E_n = \langle V \rangle$ is incorrect. The correct relation is $E_n = \frac{1}{2}\langle V \rangle$, a direct result of applying the virial theorem to the inverse-square Coulomb potential.

70 Calculate the zero-point energy for a particle in an infinite potential well for the following cases: (i) a 100 g ball confined on a 5 m long line. (ii) an oxygen atom confined to a 2×10^{-1} m lattice. (iii) an electron confined to a 10^{-10} m atom. Why zero point energy is not important for macroscopic objects? Comment.

Introduction: This problem requires calculating the zero-point energy (the ground state energy) for a particle confined in a one-dimensional infinite potential well (also known as a particle in a box). The formula for the ground state energy is given by:

$$E_1 = \frac{h^2}{8mL^2}$$

where h is Planck's constant ($h = 6.626 \times 10^{-34}$ J·s), m is the mass of the particle, and L is the width of the potential well.

We will calculate this for:

(i) A 100 g (0.1 kg) ball confined in a 5 m long box.

(ii) An oxygen atom ($m \approx 2.66 \times 10^{-26}$ kg) in a 0.2 m box.

(iii) An electron ($m_e = 9.11 \times 10^{-31}$ kg) in a 10^{-10} m box.

Solution:

Case (i): 100 g ball in a 5 m line

Given: $m = 0.1\,\text{kg}$, $L = 5\,\text{m}$

$$E_1 = \frac{(6.626 \times 10^{-34})^2}{8 \times 0.1 \times (5)^2} = \frac{4.39 \times 10^{-67}}{8 \times 0.1 \times 25} = \frac{4.39 \times 10^{-67}}{20} = 2.195 \times 10^{-68}\,\text{J}$$

Case (ii): Oxygen atom in a 0.2 m lattice

Given: $m = 2.66 \times 10^{-26}\,\text{kg}$, $L = 0.2\,\text{m}$

$$E_1 = \frac{(6.626 \times 10^{-34})^2}{8 \times 2.66 \times 10^{-26} \times (0.2)^2} = \frac{4.39 \times 10^{-67}}{8 \times 2.66 \times 10^{-26} \times 0.04} = \frac{4.39 \times 10^{-67}}{8.51 \times 10^{-27}} \approx 5.16 \times 10^{-41}\,\text{J}$$

Case (iii): Electron in a 10^{-10} m atom

Given: $m = 9.11 \times 10^{-31}\,\text{kg}$, $L = 10^{-10}\,\text{m}$

$$E_1 = \frac{(6.626 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times (10^{-10})^2} = \frac{4.39 \times 10^{-67}}{8 \times 9.11 \times 10^{-31} \times 10^{-20}} = \frac{4.39 \times 10^{-67}}{7.29 \times 10^{-50}} \approx 6.02 \times 10^{-18}\,\text{J}$$

Converting to electronvolts:

$$E_1 \approx \frac{6.02 \times 10^{-18}}{1.602 \times 10^{-19}} \approx 37.6\,\mathrm{eV}$$

Comment on Macroscopic Objects:

The zero-point energy for macroscopic objects such as a 100 g ball is extremely small ($\sim 10^{-68}$ J), far below any measurable energy scale and thus negligible. In contrast, quantum systems like electrons exhibit zero-point energies comparable to their interaction energies. Therefore, quantum effects like zero-point energy are only significant for microscopic particles where the product mL^2 is sufficiently small.

Conclusion:

(i) Zero-point energy of 100 g ball in 5 m box: 2.2×10^{-68} J

(ii) Zero-point energy of oxygen atom in 0.2 m lattice: 5.2×10^{-40} J

(iii) Zero-point energy of electron in 10^{-10} m atom: 6.02×10^{-18} J or $37.6\,\mathrm{eV}$

Zero-point energy is negligible for macroscopic systems but crucial in microscopic quantum systems due to the inverse dependence on mass and confinement size.