



UPSC PHYSICS OPTIONAL

Quantum Mechanics Solutions

PART 1 7



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UPSC PHYSICS PYQ SOLUTION

Quantum Mechanics - Part 1 to 7

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Why zero point energy is not important for macroscopic objects?

Comment.

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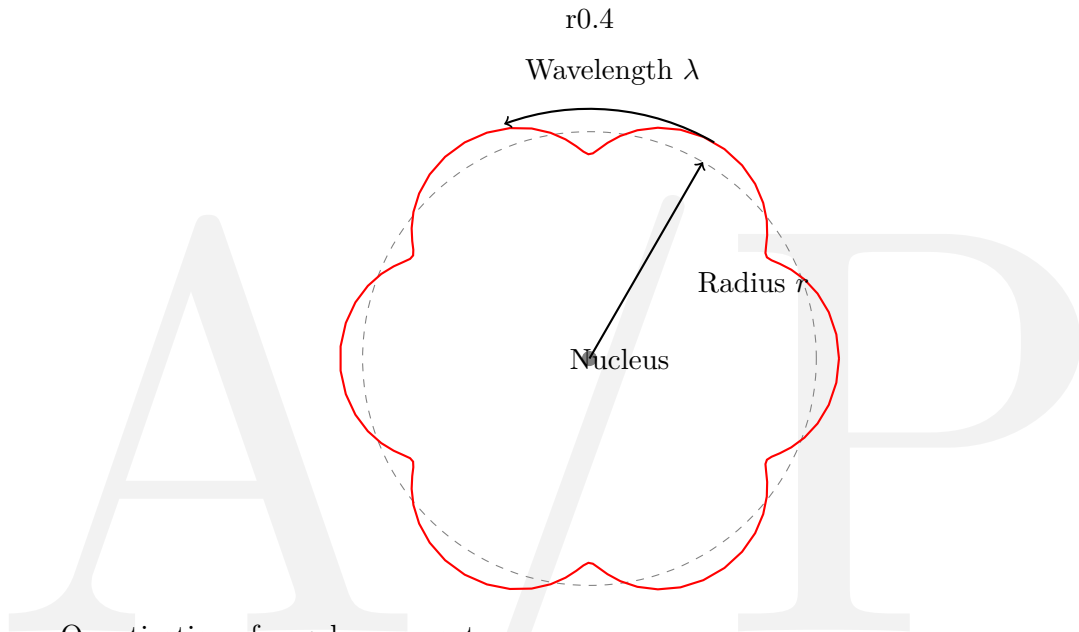
1 Derive Bohr's angular momentum quantization condition in Bohr's atomic model from the concept of de Broglie waves. (2010)

Introduction: Bohr's atomic model introduces the concept of quantized angular momentum for electrons orbiting the nucleus. This concept is fundamentally linked to the wave nature of electrons as described by de Broglie.

Solution: According to de Broglie, the wavelength of an electron is given by:

$$\lambda = \frac{h}{p}$$

where h is Planck's constant and p is the momentum of the electron.



Quantization of angular momentum

For an electron in a circular orbit of radius r , the circumference must be an integral multiple of the de Broglie wavelength:

$$2\pi r = n\lambda$$

Substituting the de Broglie wavelength:

$$2\pi r = n \frac{h}{p}$$

Since $p = mv$ for an electron of mass m and velocity v :

$$2\pi r = n \frac{h}{mv}$$

Rearranging for the angular momentum L :

$$L = mvr = n \frac{h}{2\pi}$$

Thus, the angular momentum is quantized:

$$L = n\hbar$$

where $\hbar = \frac{h}{2\pi}$.

Conclusion: Bohr's quantization of angular momentum provides a fundamental insight into the discrete nature of atomic energy levels, leading to the explanation of atomic spectra.

2 Calculate the wavelength of de Broglie waves associated with electrons accelerated through a potential difference of 200 Volts. (2011)

Introduction: The concept of de Broglie wavelength states that a particle also behaves as a wave, whose wavelength can be calculated when they are accelerated by a known potential difference.

Solution: The kinetic energy gained by the electron is:

$$eV = \frac{1}{2}mv^2$$

where e is the electron charge, V is the potential difference, m is the electron mass, and v is the velocity.

Rearranging for v :

$$v = \sqrt{\frac{2eV}{m}}$$

The de Broglie wavelength is given by:

$$\lambda = \frac{h}{mv}$$

Substituting v :

$$\lambda = \frac{h}{m\sqrt{\frac{2eV}{m}}} = \frac{h}{\sqrt{2meV}}$$

Using $h = 6.626 \times 10^{-34}$ Js, $m = 9.109 \times 10^{-31}$ kg, and $e = 1.602 \times 10^{-19}$ C:

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.109 \times 10^{-31} \times 1.602 \times 10^{-19} \times 200}}$$

$$\lambda \approx 8.6 \times 10^{-12} \text{ meters}$$

Conclusion: The wavelength of de Broglie waves associated with electrons accelerated through 200 Volts is approximately 8.6×10^{-12} meters, which highlights the wave nature of electrons at the atomic scale.

3 Estimate the size of the hydrogen atom and the ground state energy from the uncertainty principle. (2012)

Introduction: We aim to estimate the characteristic size of the hydrogen atom and its ground state energy using Heisenberg's uncertainty principle. We will model the electron bound to the proton via Coulomb attraction, and apply quantum mechanical uncertainty relations to find approximate expressions for both the radius and the minimum energy of the electron in its ground state.

Given:

We estimate the electrons position uncertainty as the size of the atom r , and relate the momentum uncertainty Δp via the uncertainty relation $\Delta x \Delta p \sim \hbar$.

Solution:

From the uncertainty principle:

$$\Delta x \Delta p \sim \hbar \Rightarrow \Delta p \sim \frac{\hbar}{r}$$

Assuming $\Delta p \sim p$, we estimate the kinetic energy as:

$$K \sim \frac{p^2}{2m_e} \sim \frac{\hbar^2}{2m_e r^2}$$

The potential energy due to the Coulomb attraction between electron and proton is:

$$U \sim -\frac{k_e e^2}{r}$$

Hence, the total energy is approximately:

$$E(r) \sim \frac{\hbar^2}{2m_e r^2} - \frac{k_e e^2}{r}$$

To find the equilibrium (minimum energy), we differentiate $E(r)$ with respect to r and set to zero:

$$\frac{dE}{dr} = -\frac{\hbar^2}{m_e r^3} + \frac{k_e e^2}{r^2} = 0$$

Solving:

$$\frac{\hbar^2}{m_e r^3} = \frac{k_e e^2}{r^2} \Rightarrow r = \frac{\hbar^2}{m_e k_e e^2}$$

Substituting values:

$$r = \frac{(1.05 \times 10^{-34})^2}{(9.11 \times 10^{-31})(8.99 \times 10^9)(1.60 \times 10^{-19})^2}$$

Calculating:

$$\begin{aligned} r &\approx \frac{1.10 \times 10^{-68}}{(9.11 \times 10^{-31})(8.99 \times 10^9)(2.56 \times 10^{-38})} \\ &\approx \frac{1.10 \times 10^{-68}}{2.09 \times 10^{-58}} \\ &\approx 5.26 \times 10^{-11} \text{ m} \end{aligned}$$

This is approximately the Bohr radius.

Now substitute r back into $E(r)$ to get the ground state energy:

$$E \approx \frac{\hbar^2}{2m_e r^2} - \frac{k_e e^2}{r}$$

Compute each term:

$$\begin{aligned}\frac{\hbar^2}{2m_e r^2} &\approx \frac{1.10 \times 10^{-68}}{2 \cdot 9.11 \times 10^{-31} \cdot (5.26 \times 10^{-11})^2} \approx 2.18 \times 10^{-18} \text{ J} \\ \frac{k_e e^2}{r} &\approx \frac{8.99 \times 10^9 \cdot (1.60 \times 10^{-19})^2}{5.26 \times 10^{-11}} \approx 4.36 \times 10^{-18} \text{ J}\end{aligned}$$

Thus,

$$E \approx 2.18 \times 10^{-18} - 4.36 \times 10^{-18} = -2.18 \times 10^{-18} \text{ J}$$

Convert to electronvolts:

$$E \approx \frac{-2.18 \times 10^{-18} \text{ J}}{1.60 \times 10^{-19} \text{ J/eV}} \approx -13.6 \text{ eV}$$

Conclusion:

Using the uncertainty principle, we estimate:

- The size (radius) of the hydrogen atom: $r \approx 5.26 \times 10^{-11} \text{ m}$ (Bohr radius)
- The ground state energy: $E_0 \approx -13.6 \text{ eV}$

These estimates agree remarkably well with the results from the full quantum mechanical treatment of the hydrogen atom, illustrating the power of the uncertainty principle in deriving fundamental atomic properties.

4 Use the uncertainty principle to estimate the ground state energy of a linear harmonic oscillator. (2012)

Introduction: The uncertainty principle, formulated by Werner Heisenberg, states that two conjugate pair (which do not commute) in quantum mechanics can never be precisely measured simultaneously. In this case it states that energy and time can't be exactly determined simultaneously.

Solution: For a harmonic oscillator, the potential energy is given by:

$$V(x) = \frac{1}{2}kx^2$$

The total energy E in the ground state is:

$$E = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

Using the uncertainty principle $\Delta x \Delta p \geq \frac{\hbar}{2}$, we set $\Delta p \approx p$ and $\Delta x \approx x$:

$$x \cdot p \geq \frac{\hbar}{2} \Rightarrow p \geq \frac{\hbar}{2x}$$

Substituting into the energy expression:

$$E \geq \frac{(\hbar/2x)^2}{2m} + \frac{1}{2}kx^2$$

Minimizing E with respect to x :

$$E = \frac{\hbar^2}{8mx^2} + \frac{1}{2}kx^2$$

Setting the derivative $\frac{dE}{dx} = 0$:

$$-\frac{\hbar^2}{4mx^3} + kx = 0 \Rightarrow x^4 = \frac{\hbar^2}{4mk} \Rightarrow x^2 = \frac{\hbar}{2\sqrt{mk}}$$

Substituting x^2 back into E :

$$E = \frac{\hbar^2}{8m \cdot \frac{\hbar}{2\sqrt{mk}}} + \frac{1}{2}k \cdot \frac{\hbar}{2\sqrt{mk}}$$

$$E = \frac{\hbar\sqrt{k/m}}{4} + \frac{\hbar\sqrt{k/m}}{4} = \frac{\hbar\omega}{2}$$

where $\omega = \sqrt{k/m}$.

Conclusion: The ground state energy of a linear harmonic oscillator is $\frac{\hbar\omega}{2}$, demonstrating the **zero-point energy due to quantum fluctuations**. Because of the zero-point energy, the position and momentum of the oscillator in the ground state are not fixed (as they would be in a classical oscillator), but have a small range of variance, in accordance with the Heisenberg uncertainty principle.

5 In a series of experiments on the determination of the mass of a certain elementary particle, the results showed a variation of $\pm 20m_e$, where m_e is the electron mass. Estimate the lifetime of the particle. (2013)

Introduction: The uncertainty principle, formulated by Werner Heisenberg, states that two conjugate pair(which do not commute) in quantum mechanics can never be precisely measured simultaneously. In this case it states that energy and time cant be exactly determined simultaneously.

Solution: Given the mass uncertainty $\Delta m = \pm 20m_e$, where m_e is the electron mass, we use the energy-time uncertainty principle:

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

The energy uncertainty ΔE can be related to the mass uncertainty Δm through $E = mc^2$:

$$\Delta E = \Delta mc^2$$

Substituting $\Delta m = 40m_e$:

$$\Delta E = 40m_e c^2$$

Using the uncertainty principle:

$$40m_e c^2 \Delta t \geq \frac{\hbar}{2}$$

$$\Delta t \geq \frac{\hbar}{2 \cdot 40m_e c^2}$$

$$\Delta t \geq \frac{\hbar}{80m_e c^2}$$

Given $\hbar \approx 1.054 \times 10^{-34}$ Js and $m_e c^2 \approx 8.187 \times 10^{-14}$ J:

$$\Delta t \geq \frac{1.054 \times 10^{-34}}{80 \times 8.187 \times 10^{-14}}$$

$$\Delta t \geq 1.61 \times 10^{-23} \text{ s}$$

Conclusion: The estimated lifetime of the particle, based on its mass uncertainty, is 1.61×10^{-23} s. **It decays via a weak force into a nucleon and a pion which highlights the precision required in high-energy physics experiments and the stability of the Lambda particle.**

6 Find the de Broglie wavelength of neutron and electron with kinetic energy 500 eV. (2014)

Introduction: The de Broglie wavelength is a fundamental concept in quantum mechanics, introduced by Louis de Broglie. It describes the wave-like behavior of particles and is inversely proportional to their momentum.

Solution: For a particle, the de Broglie wavelength λ is given by:

$$\lambda = \frac{h}{p}$$

where h is Planck's constant and p is the momentum of the particle.

(i) A neutron with kinetic energy of 500 eV: The kinetic energy E_k is related to the momentum p by:

$$E_k = \frac{p^2}{2m}$$

Solving for p :

$$p = \sqrt{2mE_k}$$

Substituting $E_k = 500 \text{ eV}$ and $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$:

$$\begin{aligned} E_k &= 500 \times 1.602 \times 10^{-19} \text{ J} \\ p &= \sqrt{2 \times 1.675 \times 10^{-27} \text{ kg} \times 500 \times 1.602 \times 10^{-19} \text{ J}} \\ p &= \sqrt{2863.35 \times 10^{-46} \text{ kg} \cdot \text{m/s}} \\ p &\approx 5.3 \times 10^{-22} \text{ kg} \cdot \text{m/s} \end{aligned}$$

The de Broglie wavelength is:

$$\begin{aligned} \lambda &= \frac{6.626 \times 10^{-34} \text{ Js}}{5.3 \times 10^{-22} \text{ kg} \cdot \text{m/s}} \\ \lambda &\approx 1.28 \times 10^{-12} \text{ m} \end{aligned}$$

(ii) An electron with kinetic energy of 500 eV: The kinetic energy E_k is related to the momentum p by:

$$E_k = \frac{p^2}{2m_e}$$

Solving for p :

$$p = \sqrt{2m_e E_k}$$

Substituting $E_k = 500 \text{ eV}$ and $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$:

$$\begin{aligned} E_k &= 500 \times 1.602 \times 10^{-19} \text{ J} \\ p &= \sqrt{2 \times 9.11 \times 10^{-31} \text{ kg} \times 500 \times 1.602 \times 10^{-19} \text{ J}} \\ p &= \sqrt{1.457 \times 10^{-46} \text{ kg} \cdot \text{m/s}} \\ p &\approx 1.21 \times 10^{-23} \text{ kg} \cdot \text{m/s} \end{aligned}$$

The de Broglie wavelength is:

$$\begin{aligned} \lambda &= \frac{6.626 \times 10^{-34} \text{ Js}}{1.21 \times 10^{-23} \text{ kg} \cdot \text{m/s}} \\ \lambda &\approx 5.48 \times 10^{-11} \text{ m} \end{aligned}$$

Conclusion: The de Broglie wavelength of a neutron with kinetic energy of 500 eV is approximately 1.28×10^{-12} m, while that of an electron with the same kinetic energy is approximately 5.48×10^{-11} m. These results illustrate the wave-particle duality of matter, with significant differences in wavelengths due to the mass disparity between neutrons and electrons.

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7 The mean life of Lambda (Λ^0) particle is 2.6×10^{-10} s. What will be the uncertainty in the determination of its mass in eV? (2014)

Introduction: The uncertainty principle, formulated by Werner Heisenberg, states that two conjugate pair (which do not commute) in quantum mechanics can never be precisely measured simultaneously. In this case it states that energy and time cant be exactly determined simultaneously

Solution: Given the mean life of Lambda particle (Λ^0) is 2.6×10^{-10} s, we use the energy-time uncertainty principle:

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Rewriting in terms of mass uncertainty:

$$\Delta mc^2 \cdot \Delta t \geq \frac{\hbar}{2}$$

$$\Delta m \geq \frac{\hbar}{2c^2 \Delta t}$$

Given $\Delta t = 2.6 \times 10^{-10}$ s, $\hbar = 1.054 \times 10^{-34}$ Js, and $c = 3 \times 10^8$ m/s:

$$\Delta mc^2 \geq \frac{1.054 \times 10^{-34}}{2 \times 2.6 \times 10^{-10}}$$

$$\Delta mc^2 \geq \frac{1.054 \times 10^{-34}}{5.2 \times 10^{-10}}$$

$$\Delta E \geq 0.202 \times 10^{-24} \text{ J}$$

Converting to energy using $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$:

$$\Delta E \approx 0.202 \times 10^{-24}$$

$$\Delta E \approx 2.025 \times 10^{-25} \text{ J}$$

$$\Delta E \approx \frac{2.025 \times 10^{-25}}{1.602 \times 10^{-19}} \text{ eV}$$

$$\Delta E \approx 1.26 \times 10^{-6} \text{ eV}$$

Conclusion: The uncertainty in the mass determination of the Lambda particle is approximately 1.26×10^{-6} eV. **It decays via a weak force into a nucleon and a pion which highlights the precision required in high-energy physics experiments and the stability of the Lambda particle.**

8 Find the energy, momentum and wavelength of photon emitted by a hydrogen atom making a direct transition from an excited state with $n = 10$ to the ground state. Also find the recoil speed of the hydrogen atom in this process. (2016)

Introduction: Whenever an electron makes a transition from higher energy level to lower energy level it radiates energy in forms of quanta. The transitioned photon had a momentum and corresponding wavelength associated with it.

Solution: For an electron transitioning from $n = 10$ to the ground state ($n = 1$), the energy difference is given by:

$$E_n = -13.6 \frac{1}{n^2} \text{ eV}$$

The energy of the photon emitted:

$$\Delta E = E_1 - E_{10}$$

$$E_1 = -13.6 \text{ eV}, \quad E_{10} = -13.6 \frac{1}{10^2} = -0.136 \text{ eV}$$

$$\Delta E = -0.136 \text{ eV} - (-13.6 \text{ eV})$$

$$\Delta E = 13.464 \text{ eV}$$

The wavelength λ of the emitted photon:

$$E = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{\Delta E}$$

Given $h = 6.626 \times 10^{-34} \text{ Js}$, $c = 3 \times 10^8 \text{ m/s}$, and $\Delta E = 13.464 \times 1.602 \times 10^{-19} \text{ J}$:

$$\lambda = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{13.464 \times 1.602 \times 10^{-19}}$$

$$\lambda \approx 9.13 \times 10^{-8} \text{ m} \approx 91.3 \text{ nm}$$

To find the recoil speed v_r of the hydrogen atom:

$$p = \frac{E}{c} = \frac{13.464 \times 1.602 \times 10^{-19}}{3 \times 10^8} \approx 7.19 \times 10^{-27} \text{ kg} \cdot \text{m/s}$$

Using momentum conservation, $p = Mv_r$:

$$v_r = \frac{p}{M}$$

Given $M \approx 1.67 \times 10^{-27} \text{ kg}$:

$$v_r = \frac{7.19 \times 10^{-27}}{1.67 \times 10^{-27}}$$

$$v_r \approx 4.3 \text{ m/s}$$

Conclusion: The photon emitted in the hydrogen atom transition has a wavelength of 91.3 nm, and the recoil speed of the hydrogen atom is approximately 4.3 m/s. **These results illustrate the principles of energy quantization and conservation in atomic transitions, with applications in spectroscopy and quantum mechanics.**

9 An electron is confined to move between two rigid walls separated by 10^{-9} m. Compute the de Broglie wavelengths representing the first three allowed energy states of the electron and the corresponding energies. (2016)

Introduction: The de Broglie wavelength is a fundamental concept in quantum mechanics which describes the wave nature of particles. According to de Broglie's hypothesis, every moving particle or object has an associated wave. The wavelength is inversely proportional to its momentum. This concept was historically pivotal in the development of quantum mechanics.

Solution: To solve for the de Broglie wavelengths and the corresponding energies, we will use the particle in a box model. Here, the electron is confined in a one-dimensional potential well of width $L = 10^{-9}$ m.

The energy levels for a particle in a box are given by:

$$E_n = \frac{n^2 h^2}{8mL^2}$$

where: - n is the principal quantum number (1, 2, 3, ...), - h is Planck's constant, 6.626×10^{-34} Js, - m is the mass of the electron, 9.109×10^{-31} kg, - L is the width of the box.

Let's compute the first three energy levels.

For $n = 1$:

$$E_1 = \frac{1^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.109 \times 10^{-31} \times (10^{-9})^2}$$

$$E_1 = \frac{6.626^2 \times 10^{-68}}{8 \times 9.109 \times 10^{-31} \times 10^{-18}}$$

$$E_1 = \frac{43.95 \times 10^{-68}}{7.287 \times 10^{-48}}$$

$$E_1 = 6.03 \times 10^{-20} \text{ J}$$

For $n = 2$:

$$E_2 = \frac{4 \times (6.626 \times 10^{-34})^2}{8 \times 9.109 \times 10^{-31} \times (10^{-9})^2}$$

$$E_2 = 4 \times E_1$$

$$E_2 = 4 \times 6.03 \times 10^{-20}$$

$$E_2 = 2.41 \times 10^{-19} \text{ J}$$

For $n = 3$:

$$E_3 = \frac{9 \times (6.626 \times 10^{-34})^2}{8 \times 9.109 \times 10^{-31} \times (10^{-9})^2}$$

$$E_3 = 9 \times E_1$$

$$E_3 = 9 \times 6.03 \times 10^{-20}$$

$$E_3 = 5.43 \times 10^{-19} \text{ J}$$

Now, the de Broglie wavelength is given by:

$$\lambda_n = \frac{h}{p_n}$$

where p_n is the momentum of the electron in the n -th energy state. For a particle in a box, the momentum is given by:

$$p_n = \sqrt{2mE_n}$$

So, for the first three states: For $n = 1$:

$$p_1 = \sqrt{2 \times 9.109 \times 10^{-31} \times 6.03 \times 10^{-20}}$$

$$p_1 = 3.3 \times 10^{-25} \text{ kg m/s}$$

$$\lambda_1 = \frac{6.626 \times 10^{-34}}{3.3 \times 10^{-25}}$$

$$\lambda_1 = 2.007 \times 10^{-9} \text{ m}$$

For $n = 2$:

$$p_2 = \sqrt{2 \times 9.109 \times 10^{-31} \times 2.41 \times 10^{-19}}$$

$$p_2 = \sqrt{4.38 \times 10^{-49}}$$

$$p_2 = 6.6 \times 10^{-25} \text{ kg m/s}$$

$$\lambda_2 = \frac{6.626 \times 10^{-34}}{6.6 \times 10^{-25}}$$

$$\lambda_2 = 10^{-9} \text{ m}$$

For $n = 3$:

$$p_3 = \sqrt{2 \times 9.109 \times 10^{-31} \times 5.43 \times 10^{-19}}$$

$$p_3 = \sqrt{9.89 \times 10^{-49}}$$

$$p_3 = 9.94 \times 10^{-25} \text{ kg m/s}$$

$$\lambda_3 = \frac{6.626 \times 10^{-34}}{9.94 \times 10^{-25}}$$

$$\lambda_3 = 6.66 \times 10^{-10} \text{ m}$$

Wavefunctions and Energy Levels:

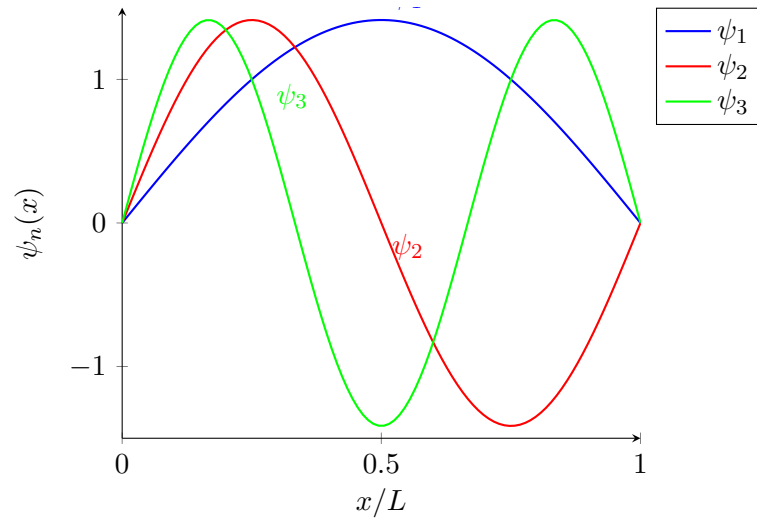


Figure 1: Wavefunctions for the first three energy states

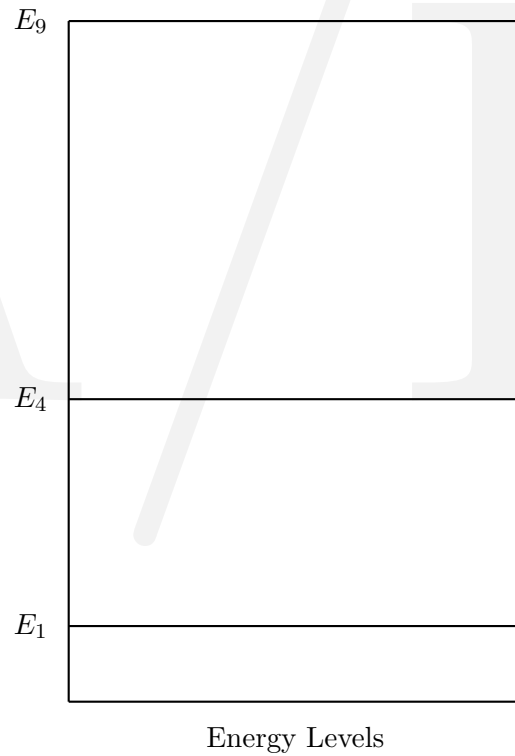


Figure 2: Energy levels for the first three states

Conclusion: These values reflect the quantized nature of energy levels in a confined system, significant in fields like **quantum computing and semiconductor physics**.

10 A typical atomic radius is about 5×10^{-15} m and the energy of β -particle emitted from a nucleus is at most of the order of 1 MeV. Prove on the basis of uncertainty principle that the electrons are not present in nuclei. (2016)

Introduction: The uncertainty principle, formulated by Werner Heisenberg, states that two conjugate pair (which do not commute) in quantum mechanics can never be precisely measured simultaneously. In this case it states that energy and time cant be exactly determined simultaneously..

Solution:

The Heisenberg Uncertainty Principle is given by:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

where Δx is the uncertainty in position and Δp is the uncertainty in momentum. Here, $\hbar$ is the reduced Planck's constant, $\hbar = \frac{h}{2\pi} \approx 1.055 \times 10^{-34}$ Js.

For an electron confined within a nucleus of radius $R \approx 5 \times 10^{-15}$ m, the uncertainty in position Δx is approximately the size of the nucleus:

$$\Delta x \approx 5 \times 10^{-15} \text{ m}$$

The uncertainty in momentum Δp can be found using the uncertainty principle:

$$\Delta p \geq \frac{\hbar}{2\Delta x}$$

Substituting the values:

$$\Delta p \geq \frac{1.055 \times 10^{-34}}{2 \times 5 \times 10^{-15}}$$

$$\Delta p \geq \frac{1.055 \times 10^{-34}}{10 \times 10^{-15}}$$

$$\Delta p \geq 1.055 \times 10^{-20} \text{ kg m/s}$$

The kinetic energy E of an electron can be related to its momentum p by the non-relativistic formula:

$$E = \frac{p^2}{2m}$$

where m is the mass of the electron, $m \approx 9.109 \times 10^{-31}$ kg. Using Δp for p :

$$E \geq \frac{(1.055 \times 10^{-20})^2}{2 \times 9.109 \times 10^{-31}}$$

$$E \geq \frac{1.113 \times 10^{-40}}{1.822 \times 10^{-30}}$$

$$E \geq 6.11 \times 10^{-11} \text{ J}$$

Converting this energy into electron volts ($1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$):

$$E \geq \frac{6.11 \times 10^{-11}}{1.602 \times 10^{-19}} \text{ eV}$$

$$E \geq 3.81 \times 10^8 \text{ eV}$$

$$E \geq 381 \text{ MeV}$$

Conclusion: The minimum energy of an electron confined within a nucleus, according to the uncertainty principle, is approximately 381 MeV. This is significantly higher than the typical energy of β -particles emitted from a nucleus, which is about 1 MeV. Thus, electrons cannot be present in the nucleus as their confinement would require them to possess unreasonably high energy, inconsistent with observed nuclear phenomena.

A/P

11 A beam 4.0 keV electrons from a source is incident on a target 50.0 cm away. Find the radius of the electron beam spot due to Heisenberg's uncertainty principle. (2017)

Introduction: The uncertainty principle, formulated by Werner Heisenberg, states that the position and momentum of a particle cannot be simultaneously determined with arbitrary precision. For an electron beam, this principle limits how tightly the beam can be focused, leading to a minimum spot size on the target. And additionally it could be interpreted as a beam of electrons which is moving along a specified direction and it encounters a diaphragm with a slit and for that reason electrons under go diffraction.

Solution:

Given:

- Energy of electrons, $E = 4.0 \text{ keV} = 4.0 \times 10^3 \times 1.602 \times 10^{-19} \text{ J} = 6.408 \times 10^{-16} \text{ J}$
- Distance to target, $L = 50.0 \text{ cm} = 0.50 \text{ m}$

Verification: Check if non-relativistic approximation is valid

The electron velocity is:

$$v = \frac{p}{m} = \frac{3.42 \times 10^{-23}}{9.109 \times 10^{-31}} = 3.75 \times 10^7 \text{ m/s}$$

Since $v/c = 3.75 \times 10^7 / (3 \times 10^8) = 0.125 < 0.3$, the non-relativistic approximation is reasonable.

For non-relativistic electrons, the kinetic energy E is related to momentum by:

$$E = \frac{p^2}{2m}$$

where $m = 9.109 \times 10^{-31} \text{ kg}$ is the electron mass.

Solving for momentum:

$$p = \sqrt{2mE}$$

Substituting values:

$$p = \sqrt{2 \times 9.109 \times 10^{-31} \times 6.408 \times 10^{-16}}$$
$$p = \sqrt{1.167 \times 10^{-45}} = 3.42 \times 10^{-23} \text{ kgm/s}$$

The uncertainty principle states:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

where $\hbar = 1.055 \times 10^{-34} \text{ Js}$.

For minimum uncertainty (equality case):

$$\Delta x = \frac{\hbar}{2\Delta p}$$

If the initial beam has an uncertainty in transverse position Δx_0 , then by the uncertainty principle, it must have a corresponding uncertainty in transverse momentum:

$$\Delta p_{\perp} \geq \frac{\hbar}{2\Delta x_0}$$

This transverse momentum uncertainty causes the beam to spread as it travels. The angular divergence is:

$$\theta \approx \frac{\Delta p_{\perp}}{p} = \frac{\hbar}{2\Delta x_0 \cdot p}$$

As the beam travels distance L , the radius of the spot becomes:

$$r = \Delta x_0 + L \cdot \theta = \Delta x_0 + L \cdot \frac{\hbar}{2\Delta x_0 \cdot p}$$

To minimize the spot size (as we want to ascertain the spot to be definite or you might think the radius from center to the first minima of the diffraction pattern), we differentiate with respect to Δx_0 and set equal to zero:

$$\frac{dr}{d\Delta x_0} = 1 - \frac{L\hbar}{2(\Delta x_0)^2 p} = 0$$

This gives the optimal initial beam width:

$$\Delta x_0 = \sqrt{\frac{L\hbar}{2p}}$$

The minimum spot radius is:

$$r = r_{min} = \Delta x_0 + L \cdot \theta = \Delta x_0 + L \cdot \frac{\hbar}{2\Delta x_0 \cdot p}$$

$$\begin{aligned} r_{min} &= \sqrt{\frac{L\hbar}{2p}} + \frac{L\hbar}{2p \cdot \sqrt{\frac{L\hbar}{2p}}} \\ &= \sqrt{\frac{L\hbar}{2p}} + \sqrt{\frac{L\hbar}{2p}} \\ &= 2\sqrt{\frac{L\hbar}{2p}} \\ &= \sqrt{\frac{2L\hbar}{p}} \end{aligned}$$

Substituting the values:

$$\begin{aligned} r_{min} &= \sqrt{\frac{2L\hbar}{p}} \\ &= \sqrt{\frac{2 \cdot 0.50 \cdot 1.055 \times 10^{-34}}{3.42 \times 10^{-23}}} \\ &= \sqrt{3.08 \times 10^{-12}} \\ &= 1.76 \times 10^{-6} \text{ m} \\ &\approx \boxed{1.8 \mu\text{m}} \end{aligned}$$

Therefore:

$$r_{\min} \approx 1.8 \times 10^{-6} \text{ m} = 1.8\mu\text{m}$$

Conclusion: The minimum radius of the electron beam spot on the target due to Heisenberg's uncertainty principle is approximately $1.8\mu\text{m}$. This fundamental quantum mechanical limit demonstrates why electron microscopes and other high-precision electron beam instruments face ultimate resolution limits determined by the uncertainty principle.

A/P

12 Estimate the de Broglie wavelength of the electron orbiting in the first excited state of the hydrogen atom. (2017)

Introduction:

The de Broglie wavelength is a fundamental concept in quantum mechanics that describes the wave-like behavior of particles. Introduced by Louis de Broglie in 1924, it posits that any moving particle has an associated wavelength given by $\lambda = \frac{h}{p}$, where h is Planck's constant and p is the particle's momentum. This principle bridges classical and quantum mechanics, highlighting the wave-particle duality of matter.

Solution:

We can also determine the de Broglie wavelength of the electron using the energy of the first excited state of the hydrogen atom. The total energy of an electron in the n -th orbit is given by:

$$E_n = -\frac{13.6 \text{ eV}}{n^2}$$

For the first excited state ($n = 2$):

$$E_2 = -\frac{13.6 \text{ eV}}{2^2} = -\frac{13.6 \text{ eV}}{4} = -3.4 \text{ eV}$$

This energy is the sum of the kinetic and potential energies. In the Bohr model of the hydrogen atom, the kinetic energy (K.E.) is equal to the negative of the total energy:

$$\text{K.E.} = -E_2 = 3.4 \text{ eV}$$

To find the momentum p of the electron, we use the relation between kinetic energy and momentum:

$$\text{K.E.} = \frac{p^2}{2m}$$

Solving for p :

$$p = \sqrt{2m \cdot \text{K.E.}}$$

Converting the kinetic energy to joules:

$$3.4 \text{ eV} = 3.4 \times 1.602 \times 10^{-19} \text{ J} = 5.447 \times 10^{-19} \text{ J}$$

Now, substituting the mass of the electron $m = 9.109 \times 10^{-31} \text{ kg}$:

$$p = \sqrt{2 \cdot 9.109 \times 10^{-31} \text{ kg} \cdot 5.447 \times 10^{-19} \text{ J}}$$

$$p = \sqrt{9.919 \times 10^{-49} \text{ kg}^2 \cdot \text{m}^2 \cdot \text{s}^{-2}}$$

$$p \approx 9.96 \times 10^{-25} \text{ kg m/s}$$

Finally, we calculate the de Broglie wavelength λ :

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34} \text{ Js}}{9.96 \times 10^{-25} \text{ kg m/s}}$$

$$\lambda \approx 6.65 \times 10^{-10} \text{ m}$$

$$\lambda \approx 0.665 \text{ nm}$$

Conclusion:

The de Broglie wavelength of the electron in the first excited state of the hydrogen atom is approximately 0.665 nm. This wavelength reflects the wave-particle duality of the electron, emphasizing its quantum mechanical nature. Such insights are crucial for understanding phenomena at atomic scales, including electron diffraction and the formation of atomic spectra.

A/P

13 Show that the mass and linear momentum of a quantum mechanical particle can be given by $m = \frac{h}{\lambda v}$ and $p = \frac{h}{\lambda}$, respectively, where h, λ and v are Planck's constant, wavelength, and velocity of the particle, respectively. Comment on the wave-particle duality from these relations. (2019)

Introduction:

The de Broglie hypothesis posits that every moving particle has an associated wavelength, bridging the gap between classical and quantum physics. This hypothesis, introduced by Louis de Broglie in 1924, demonstrates the wave-particle duality, a cornerstone of quantum mechanics.

Solution:

To show the given relations, we start from the de Broglie wavelength formula. The de Broglie wavelength λ is given by:

$$\lambda = \frac{h}{p}$$

where h is Planck's constant and p is the momentum of the particle.

1. Derivation of momentum: Given the de Broglie relation:

$$\lambda = \frac{h}{p}$$

Solving for p :

$$p = \frac{h}{\lambda}$$

2. Derivation of mass: We also know that momentum p is related to mass m and velocity v by:

$$p = mv$$

Substituting $p = \frac{h}{\lambda}$ from the de Broglie relation:

$$mv = \frac{h}{\lambda}$$

Solving for m :

$$m = \frac{h}{\lambda v}$$

These derivations show that the mass and momentum of a quantum mechanical particle can be expressed in terms of Planck's constant, the particle's wavelength, and its velocity.

Comment on Wave-Particle Duality:

The derived relations $m = \frac{h}{\lambda v}$ and $p = \frac{h}{\lambda}$ underscore the wave-particle duality of matter. They reveal that the properties traditionally associated with particles (mass and momentum) can be described using wave characteristics (wavelength). This duality is fundamental in quantum mechanics, explaining phenomena such as electron diffraction and the quantization of atomic orbits.

Conclusion:

The expressions for mass and momentum derived from the de Broglie wavelength highlight the intrinsic connection between wave and particle properties in quantum mechanics. This wave-particle duality is crucial for understanding various quantum phenomena and has practical applications in fields like **electron microscopy and semiconductor technology**.

A/P

14 State and express mathematically the three uncertainty principles of Heisenberg. Highlight the physical significance of these principles in the development of Quantum Mechanics. (2019)

Introduction:

The Heisenberg uncertainty principle is a fundamental concept in quantum mechanics, formulated by Werner Heisenberg in 1927. It states that certain pairs of physical properties, known as **conjugate pairs**, **cannot both be known to arbitrary precision simultaneously**. This principle is mathematically expressed using the commutator of these conjugate pairs, which is non-zero.

Solution:

Heisenberg's uncertainty principle can be expressed mathematically for three different pairs of conjugate variables:

1. Position and Momentum:

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

The commutator for position $\hat{x}$ and momentum $\hat{p}$ is $[\hat{x}, \hat{p}] = i\hbar$. Since this commutator is not zero, it implies that position and momentum cannot be simultaneously determined with arbitrary precision.

2. Energy and Time:

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

The commutator for energy $\hat{E}$ and time $\hat{t}$ is $[\hat{E}, \hat{t}] = i\hbar$. This non-zero commutator signifies that energy and time cannot both be precisely measured at the same time.

3. Angular Position and Angular Momentum:

$$\Delta \theta \Delta L \geq \frac{\hbar}{2}$$

The commutator for angular position $\hat{\theta}$ and angular momentum $\hat{L}$ is $[\hat{\theta}, \hat{L}] = i\hbar$. Again, the non-zero commutator indicates that angular position and angular momentum cannot be simultaneously determined with arbitrary precision.

These inequalities show that increasing the precision in measuring one quantity leads to increased uncertainty in the conjugate quantity.

Physical Significance:

The uncertainty principles have several significant implications:

1. Limits of Measurement: They set fundamental limits on the precision of measurements, illustrating that there is a limit to how precisely we can simultaneously know certain pairs of properties of a quantum system.

2. Wave-Particle Duality: These principles highlight the wave-particle duality of matter, emphasizing that particles exhibit both wave-like and particle-like properties, depending on the measurement context.

3. Quantum Behavior: The principles help explain why atoms do not collapse, as electrons cannot have both a well-defined position and momentum. This results in stable atomic structures.

4. **Quantum Fluctuations:** In fields such as quantum field theory, the energy-time uncertainty principle is crucial for understanding quantum fluctuations and the creation of particle-antiparticle pairs.

Conclusion:

Heisenberg's uncertainty principles are cornerstones of quantum mechanics, fundamentally altering our understanding of measurement and the behavior of particles at microscopic scales. They underscore the intrinsic limitations of classical concepts when applied to quantum systems and have wide-ranging applications in technology and theoretical physics, such as in the development of quantum computers and the study of fundamental particles.

A/P

15 For a free quantum mechanical particle under the influence of a one-dimensional potential, show that the energy is quantized in discrete fashion. How do these energy values differ from those of a linear harmonic oscillator? (2019)

Introduction:

Quantum mechanics reveals that particles can only occupy certain discrete energy levels, a phenomenon known as quantization. This concept was developed in the early 20th century by scientists like Planck, Bohr, and Schrödinger. Quantization arises due to boundary conditions and the wave nature of particles.

Solution:

To show the quantization of energy, we consider a particle in a one-dimensional potential well (infinite potential well) of width L .

The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

For a particle in an infinite potential well, the potential $V(x)$ is:

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

Inside the well, the Schrödinger equation simplifies to:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

Let $k^2 = \frac{2mE}{\hbar^2}$, then:

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

The general solution to this differential equation is:

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

Applying boundary conditions $\psi(0) = 0$ and $\psi(L) = 0$: 1. At $x = 0$:

$$\psi(0) = A \sin(0) + B \cos(0) = B = 0$$

So, $\psi(x) = A \sin(kx)$.

2. At $x = L$:

$$\psi(L) = A \sin(kL) = 0$$

Since $A \neq 0$, we must have $\sin(kL) = 0$.

Thus, $kL = n\pi$, where n is an integer ($n = 1, 2, 3, \dots$).

So, $k = \frac{n\pi}{L}$.

The energy levels are given by:

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L} \right)^2 = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

Hence, the energy is quantized and the allowed energies are:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{for } n = 1, 2, 3, \dots$$

Comparison with Linear Harmonic Oscillator:

For a linear harmonic oscillator, the energy levels are given by:

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega \quad \text{for } n = 0, 1, 2, \dots$$

The key differences are:

1. The energy levels for the particle in a potential well are proportional to n^2 , while for the harmonic oscillator they are proportional to $n + \frac{1}{2}$.
2. The spacing between energy levels in the potential well increases with n , whereas for the harmonic oscillator, the spacing between adjacent energy levels is constant ($\hbar \omega$).
3. There is no zero point energy in case of 1D infinite well as is the case with harmonic oscillator.
4. There is fixed boundary condition in case of infinite well i.e 0 to L but for harmonic oscillator there is a restoring force but no fixed spatial boundary condition due to which they have different energy level properties.

Conclusion:

The quantization of energy in a one-dimensional potential well demonstrates how boundary conditions lead to discrete energy levels. This concept is foundational in quantum mechanics, affecting phenomena like electron configurations in atoms and the behavior of particles in confined spaces. The comparison with the linear harmonic oscillator highlights the diversity in quantum systems, each with unique energy quantization characteristics.

16 Using the uncertainty principle $\Delta x \Delta p \geq \hbar/2$, estimate the ground state energy of a harmonic oscillator. (2020)

Introduction: The uncertainty principle, formulated by Werner Heisenberg in 1927, states that it is impossible to simultaneously determine the exact position and momentum of a particle. This principle is fundamental to quantum mechanics and impacts the behavior of quantum systems such as the harmonic oscillator.

Solution:

The ground state energy of a harmonic oscillator can be estimated using the uncertainty principle. For a harmonic oscillator, the potential energy $V(x) = \frac{1}{2}m\omega^2 x^2$ and the kinetic energy $T(p) = \frac{p^2}{2m}$.

Using the uncertainty principle $\Delta x \Delta p \geq \frac{\hbar}{2}$:

$$\Delta p \approx \frac{\hbar}{2\Delta x}$$

The total energy E is given by the sum of kinetic and potential energies. Assuming Δx is of the order of the position uncertainty and Δp is of the order of the momentum uncertainty:

$$E \approx \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$$

Substituting Δp :

$$E \approx \frac{\left(\frac{\hbar}{2\Delta x}\right)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$$

$$E \approx \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2$$

Minimizing this energy with respect to Δx , we set the derivative with respect to Δx to zero:

$$\frac{dE}{d(\Delta x)} = -\frac{\hbar^2}{4m(\Delta x)^3} + m\omega^2(\Delta x) = 0$$

$$-\frac{\hbar^2}{4m(\Delta x)^3} + m\omega^2(\Delta x) = 0$$

$$\frac{\hbar^2}{4m^2(\Delta x)^4} = \omega^2$$

$$(\Delta x)^4 = \frac{\hbar^2}{4m^2\omega^2}$$

$$(\Delta x)^2 = \frac{\hbar}{2m\omega}$$

$$\Delta x = \sqrt{\frac{\hbar}{2m\omega}}$$

Substituting back into the energy expression:

$$E \approx \frac{\hbar^2}{8m} \left(\frac{2m\omega}{\hbar} \right) + \frac{1}{2} m \omega^2 \left(\frac{\hbar}{2m\omega} \right)$$

$$E \approx \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

Thus, the ground state energy is:

$$E_0 = \frac{\hbar\omega}{2}$$

Conclusion:

The uncertainty principle is crucial in understanding the limitations of measurements at the quantum level. The calculated ground state energy of a harmonic oscillator being $\frac{\hbar\omega}{2}$ signifies the zero-point energy, indicating that even at absolute zero, the oscillator retains quantum mechanical motion. This concept is widely applicable in fields like quantum field theory and low-temperature physics.

17 A blue lamp emits light of mean wavelength of 4500 Å. The rating of the lamp is 150 W and its 8% of the energy appears as light. How many photons are emitted per second by the lamp? (2020)

Introduction: Photon emission from light sources can be quantified using the energy-wavelength relationship for photons. This relationship is fundamental in quantum mechanics and is instrumental in understanding light sources.

Solution:

First, convert the wavelength from angstroms to meters:

$$\lambda = 4500 \text{ Å} = 4500 \times 10^{-10} \text{ m} = 4.5 \times 10^{-7} \text{ m}$$

The energy of one photon E is given by:

$$E = \frac{hc}{\lambda}$$

where h is Planck's constant ($6.626 \times 10^{-34} \text{ Js}$) and c is the speed of light ($3 \times 10^8 \text{ m/s}$).

$$E = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{4.5 \times 10^{-7}} = \frac{19.878 \times 10^{-26}}{4.5 \times 10^{-7}} = 4.417 \times 10^{-19} \text{ J}$$

The power output of the lamp as light is 8% of 150 W:

$$P = 0.08 \times 150 = 12 \text{ W}$$

The number of photons emitted per second N is given by:

$$N = \frac{P}{E} = \frac{12}{4.417 \times 10^{-19}} = 2.717 \times 10^{19}$$

Thus, the number of photons emitted per second by the lamp is:

$$N \approx 2.72 \times 10^{19} \text{ photons/s}$$

Conclusion:

Photon emission quantification allows for precise control and application in various technologies such as lasers, LEDs, and other optical devices. The calculation of photon emission rate is crucial in designing efficient lighting systems and understanding the energy efficiency of light sources.

18 Consider a Hermitian operator A with property $A^3 = 1$. Show that $A = 1$. (2020)

Introduction: Hermitian operators play a critical role in quantum mechanics, especially because their eigenvalues are real. The problem explores the properties of a specific Hermitian operator.

Solution:

Given that A is a Hermitian operator, all its eigenvalues are real. Let λ be an eigenvalue of A with an eigenvector $|\psi\rangle$, i.e.,

$$A|\psi\rangle = \lambda|\psi\rangle$$

Given $A^3 = 1$,

$$A^3|\psi\rangle = 1|\psi\rangle$$

$$\lambda^3|\psi\rangle = |\psi\rangle$$

$$\lambda^3 = 1$$

The real solutions to $\lambda^3 = 1$ are $\lambda = 1$. Hence, the only eigenvalue of A is 1.

Since A is Hermitian and all its eigenvalues are 1, we can write:

$$A = I$$

Therefore,

$$A = 1$$

Conclusion:

Hermitian operators are fundamental in ensuring that measurements in quantum mechanics yield real values. The result demonstrates the specific behavior of a Hermitian operator with a given property, reinforcing the concept that such operators have real eigenvalues, which in this case leads to a unique solution. This concept has applications in quantum computing and spectral theory.

- 19 Find the uncertainty in the momentum of a particle when its position is determined within 0.02 cm. Find also the uncertainty in the velocity of an electron and α -particle respectively when they are located within 15×10^{-8} cm. (2020)**

Introduction:

The Heisenberg uncertainty principle states that it is impossible to simultaneously determine the exact position and momentum of a particle. This principle is fundamental to quantum mechanics and provides limits on how precisely we can measure these quantities.

Solution:

The uncertainty principle is given by:

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

First, let's find the uncertainty in momentum Δp when the position $\Delta x = 0.02 \text{ cm} = 0.02 \times 10^{-2} \text{ m}$.

$$\Delta p \geq \frac{\hbar}{2\Delta x}$$

Using $\hbar = 1.054 \times 10^{-34} \text{ Js}$,

$$\Delta p \geq \frac{1.054 \times 10^{-34}}{2 \times 0.02 \times 10^{-2}} \approx 2.635 \times 10^{-32} \text{ kg m/s}$$

Now, let's find the uncertainty in velocity Δv for an electron and an α -particle when the position $\Delta x = 15 \times 10^{-8} \text{ cm} = 15 \times 10^{-10} \text{ m}$.

For an electron with mass $m_e = 9.11 \times 10^{-31} \text{ kg}$,

$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{1.054 \times 10^{-34}}{2 \times 15 \times 10^{-10}} \approx 3.513 \times 10^{-26} \text{ kg m/s}$$

$$\Delta v_e \geq \frac{\Delta p}{m_e} = \frac{3.513 \times 10^{-26}}{9.11 \times 10^{-31}} \approx 3.86 \times 10^4 \text{ m/s}$$

For an α -particle with mass $m_\alpha = 4 \times 1.66 \times 10^{-27} \text{ kg} = 6.64 \times 10^{-27} \text{ kg}$,

$$\Delta v_\alpha \geq \frac{\Delta p}{m_\alpha} = \frac{3.513 \times 10^{-26}}{6.64 \times 10^{-27}} \approx 5.29 \times 10^0 \text{ m/s}$$

Conclusion: The uncertainty in the momentum of a particle when its position is determined within 0.02 cm is approximately $2.635 \times 10^{-32} \text{ kg m/s}$. For an electron and an α -particle located within $15 \times 10^{-8} \text{ cm}$, the uncertainties in their velocities are approximately $3.86 \times 10^4 \text{ m/s}$ and 5.29 m/s , respectively. This illustrates the significant impact of particle mass on the uncertainty in velocity, highlighting the precision limitations inherent in quantum measurements.

20 A particle of rest mass m_0 has a kinetic energy K , show that its de Broglie wavelength is given by $\lambda = \frac{hc}{\sqrt{K(K+2m_0c^2)}}$. Hence calculate the wavelength of an electron of kinetic energy 2 MeV. What will be the value of λ if $K \ll m_0c^2$? (2020)

Introduction: The de Broglie wavelength relates a particle's momentum to its wavelength, an essential concept in quantum mechanics introduced by Louis de Broglie in 1924. This concept is pivotal in understanding wave-particle duality.

Solution:

The total energy E of a particle is given by:

$$E = K + m_0c^2$$

The momentum p of the particle is related to its energy and mass by the relation:

$$E^2 = (pc)^2 + (m_0c^2)^2$$

Substituting $E = K + m_0c^2$,

$$(K + m_0c^2)^2 = (pc)^2 + (m_0c^2)^2$$

$$K^2 + 2Km_0c^2 + (m_0c^2)^2 = (pc)^2 + (m_0c^2)^2$$

Subtracting $(m_0c^2)^2$ from both sides,

$$K^2 + 2Km_0c^2 = (pc)^2$$

$$p = \frac{\sqrt{K^2 + 2Km_0c^2}}{c}$$

The de Broglie wavelength λ is given by:

$$\lambda = \frac{h}{p} = \frac{h}{\frac{\sqrt{K^2 + 2Km_0c^2}}{c}} = \frac{hc}{\sqrt{K^2 + 2Km_0c^2}}$$

Thus, the de Broglie wavelength is:

$$\lambda = \frac{hc}{\sqrt{K(K + 2m_0c^2)}}$$

Next, let's calculate the wavelength of an electron with kinetic energy $K = 2 \text{ MeV}$.

First, convert the kinetic energy to joules:

$$K = 2 \text{ MeV} = 2 \times 10^6 \times 1.602 \times 10^{-19} \text{ J} = 3.204 \times 10^{-13} \text{ J}$$

For an electron, $m_0 = 9.11 \times 10^{-31}$ kg and $c = 3 \times 10^8$ m/s.

Calculate m_0c^2 :

$$m_0c^2 = 9.11 \times 10^{-31} \times (3 \times 10^8)^2 \text{ J} = 8.2 \times 10^{-14} \text{ J}$$

Now, calculate λ :

$$\lambda = \frac{hc}{\sqrt{K(K + 2m_0c^2)}}$$

Using $h = 6.626 \times 10^{-34}$ Js,

$$\lambda = \frac{1.988 \times 10^{-25}}{\sqrt{3.204 \times 10^{-13} \times 4.844 \times 10^{-13}}}$$

$$\lambda = \frac{1.988 \times 10^{-25}}{\sqrt{1.551 \times 10^{-25}}}$$

$$\lambda = \frac{1.988 \times 10^{-25}}{1.245 \times 10^{-12}} \approx 1.597 \times 10^{-13} \text{ m}$$

For $K \ll m_0c^2$, $K + 2m_0c^2 \approx 2m_0c^2$,

$$\lambda = \frac{hc}{\sqrt{K(2m_0c^2)}} = \frac{hc}{\sqrt{2Km_0c^2}}$$

$$\lambda \approx \frac{h}{\sqrt{2m_0K}} \times \frac{c}{c} = \frac{h}{\sqrt{2m_0K}}$$

Conclusion: The derived expression for the de Broglie wavelength $\lambda = \frac{hc}{\sqrt{K(K+2m_0c^2)}}$ links a particle's kinetic energy to its wavelength, emphasizing the relationship between energy, momentum, and wavelength in quantum mechanics.

For an electron with kinetic energy of 2 MeV, the wavelength is approximately 1.597×10^{-13} m. When $K \ll m_0c^2$, the wavelength simplifies to $\lambda \approx \frac{h}{\sqrt{2m_0K}}$, highlighting the classical limit of the de Broglie wavelength.

This relation is significant in analyzing particle behavior at quantum scales, with applications in electron microscopy and particle physics.

21 What is de Broglie concept of matter wave? Evaluate de Broglie wavelength of Helium that is accelerated through 300V. (Given mass of proton = mass of neutron = 1.67×10^{-27} kg)

Introduction: The de Broglie hypothesis, proposed by Louis de Broglie in 1924, suggests that particles such as electrons have wave-like properties, characterized by a wavelength. This concept is fundamental to quantum mechanics and leads to the wave-particle duality of matter.

Solution:

The de Broglie wavelength λ of a particle is given by:

$$\lambda = \frac{h}{p}$$

where h is Planck's constant and p is the momentum of the particle.

For a particle accelerated through a potential difference V , the kinetic energy K acquired by the particle is given by:

$$K = eV$$

where e is the elementary charge (1.602×10^{-19} C).

The kinetic energy is also related to the momentum p by:

$$K = \frac{p^2}{2m}$$

Thus,

$$p = \sqrt{2mK}$$

Substituting $K = eV$,

$$p = \sqrt{2meV}$$

Therefore, the de Broglie wavelength λ is:

$$\lambda = \frac{h}{\sqrt{2meV}}$$

Given: $h = 6.626 \times 10^{-34}$ Js $e = 1.602 \times 10^{-19}$ C $m_{\text{He}} = 4 \times (1.67 \times 10^{-27} \text{ kg}) = 6.68 \times 10^{-27}$ kg $V = 300$ V

Substitute these values into the equation:

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 6.68 \times 10^{-27} \times 1.602 \times 10^{-19} \times 300}}$$

Calculate the denominator:

$$\sqrt{2 \times 6.68 \times 10^{-27} \times 1.602 \times 10^{-19} \times 300} = \sqrt{6.434 \times 10^{-23}} = 8.02 \times 10^{-12} \text{ kg m/s}$$

Now calculate the wavelength:

$$\lambda = \frac{6.626 \times 10^{-34}}{8.02 \times 10^{-12}} \approx 8.26 \times 10^{-23} \text{ m}$$

Conclusion: The de Broglie wavelength concept reveals that particles exhibit wave-like behavior, which is fundamental to quantum mechanics. For Helium ions accelerated through a potential difference of 300V, the calculated de Broglie wavelength is approximately 8.26×10^{-23} m. This demonstrates the wave-particle duality of matter, crucial in applications such as electron microscopy and quantum computing.

A/P

22 Obtain an expression for the probability current for the plane wave $\psi(x, t) = \exp[i(kx - \omega t)]$. Interpret your result.

Introduction: In quantum mechanics, the probability current is a measure of the flow of probability associated with the wave function. It is essential for understanding the conservation of probability and the behavior of quantum particles.

Solution:

The probability current $j(x, t)$ for a wave function $\psi(x, t)$ is given by:

$$j(x, t) = \frac{\hbar}{2mi} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)$$

For the plane wave $\psi(x, t) = e^{i(kx - \omega t)}$,

The complex conjugate is:

$$\psi^*(x, t) = e^{-i(kx - \omega t)}$$

First, calculate $\frac{\partial \psi}{\partial x}$:

$$\frac{\partial \psi}{\partial x} = \frac{\partial}{\partial x} e^{i(kx - \omega t)} = ik e^{i(kx - \omega t)} = ik\psi$$

Next, calculate $\frac{\partial \psi^*}{\partial x}$:

$$\frac{\partial \psi^*}{\partial x} = \frac{\partial}{\partial x} e^{-i(kx - \omega t)} = -ik e^{-i(kx - \omega t)} = -ik\psi^*$$

Substitute these into the probability current expression:

$$j(x, t) = \frac{\hbar}{2mi} (\psi^* ik\psi - \psi(-ik\psi^*))$$

$$j(x, t) = \frac{\hbar}{2mi} (ik\psi^*\psi + ik\psi\psi^*)$$

$$j(x, t) = \frac{\hbar}{2mi} (2ik|\psi|^2)$$

Since $|\psi|^2 = \psi\psi^* = 1$ for a plane wave,

$$j(x, t) = \frac{\hbar}{2mi} \times 2ik = \frac{\hbar k}{m}$$

Conclusion: The probability current for a plane wave $\psi(x, t) = \exp[i(kx - \omega t)]$ is $j = \frac{\hbar k}{m}$. This indicates a constant flow of probability in the direction of the wave vector k , reflecting the uniform motion of the quantum particle. It highlights the conservation of probability and provides insight into the dynamics of free particles in quantum mechanics.

23 A system is described by the Hamiltonian operator $H = -\frac{d^2}{dx^2} + x^2$. Show that the function $Ax \exp\left(-\frac{x^2}{2}\right)$ is an eigenfunction of H . Determine the eigenvalues of H .

Introduction: In quantum mechanics, the Hamiltonian operator represents the total energy of a system. Eigenfunctions of the Hamiltonian correspond to stationary states with definite energy, and the associated eigenvalues represent the energy levels of the system.

Solution:

Given the Hamiltonian:

$$H = -\frac{d^2}{dx^2} + x^2$$

We need to show that the function $\psi(x) = Ax \exp\left(-\frac{x^2}{2}\right)$ is an eigenfunction of H .

First, calculate $\frac{d\psi}{dx}$:

$$\psi(x) = Ax \exp\left(-\frac{x^2}{2}\right)$$

$$\frac{d\psi}{dx} = A \left(\exp\left(-\frac{x^2}{2}\right) + x \left(-x \exp\left(-\frac{x^2}{2}\right) \right) \right) = A \exp\left(-\frac{x^2}{2}\right) (1 - x^2)$$

Next, calculate $\frac{d^2\psi}{dx^2}$:

$$\frac{d^2\psi}{dx^2} = A \left(\frac{d}{dx} \left[\exp\left(-\frac{x^2}{2}\right) (1 - x^2) \right] \right)$$

$$\frac{d^2\psi}{dx^2} = A \left(-x \exp\left(-\frac{x^2}{2}\right) (1 - x^2) + \exp\left(-\frac{x^2}{2}\right) (-2x) \right)$$

$$\frac{d^2\psi}{dx^2} = A \exp\left(-\frac{x^2}{2}\right) (-x + x^3 - 2x) = A \exp\left(-\frac{x^2}{2}\right) (x^3 - 3x)$$

Now, apply the Hamiltonian operator H to $\psi(x)$:

$$H\psi(x) = -\frac{d^2\psi}{dx^2} + x^2\psi(x)$$

Substitute $\frac{d^2\psi}{dx^2}$ and $\psi(x)$:

$$H\psi(x) = -A \exp\left(-\frac{x^2}{2}\right) (x^3 - 3x) + x^2 Ax \exp\left(-\frac{x^2}{2}\right)$$

$$H\psi(x) = -A \exp\left(-\frac{x^2}{2}\right) (x^3 - 3x) + Ax^3 \exp\left(-\frac{x^2}{2}\right)$$

$$H\psi(x) = A \exp\left(-\frac{x^2}{2}\right) (-x^3 + 3x + x^3)$$

$$H\psi(x) = 3Ax \exp\left(-\frac{x^2}{2}\right)$$

Thus,

$$H\psi(x) = 3\psi(x)$$

So, $\psi(x) = Ax \exp\left(-\frac{x^2}{2}\right)$ is an eigenfunction of H with the eigenvalue $\lambda = 3$.

Conclusion: The function $\psi(x) = Ax \exp\left(-\frac{x^2}{2}\right)$ is an eigenfunction of the Hamiltonian operator $H = -\frac{d^2}{dx^2} + x^2$ with the eigenvalue $\lambda = 3$. This shows that the system described by H has a discrete energy level corresponding to this eigenfunction. Eigenfunctions and eigenvalues are crucial in quantum mechanics for determining the stationary states and energy levels of quantum systems.

A/P

24 Solve the Schrödinger equation for a particle of mass m in an infinite rectangular well defined by $V(x) = \begin{cases} 0 & ; 0 \leq x \leq L \\ \infty & ; x < 0, x > L \end{cases}$ Obtain the normalized eigenfunctions and the corresponding eigenvalues.

Introduction: The infinite potential well is a fundamental problem in quantum mechanics, illustrating the quantization of energy levels. The Schrödinger equation provides the basis for understanding the behavior of a particle in such a well.

Solution:

The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

For $0 \leq x \leq L$, $V(x) = 0$:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

Rewriting:

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x)$$

Let $k^2 = \frac{2mE}{\hbar^2}$:

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$$

The general solution is:

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

Applying boundary conditions:

1. $\psi(0) = 0$:

$$\psi(0) = A \sin(0) + B \cos(0) = B = 0$$

So, $\psi(x) = A \sin(kx)$.

2. $\psi(L) = 0$:

$$\psi(L) = A \sin(kL) = 0$$

For a non-trivial solution ($A \neq 0$):

$$\sin(kL) = 0$$

$$kL = n\pi \quad \text{where } n = 1, 2, 3, \dots$$

Thus,

$$k = \frac{n\pi}{L}$$

The corresponding energy eigenvalues are:

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L} \right)^2 = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

The normalized eigenfunctions are:

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

Normalization condition:

$$\int_0^L |\psi_n(x)|^2 dx = 1$$

$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

Using $\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}$:

$$A^2 \frac{L}{2} = 1$$

$$A^2 = \frac{2}{L}$$

$$A = \sqrt{\frac{2}{L}}$$

Thus, the normalized eigenfunctions are:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Conclusion: The solution to the Schrödinger equation for a particle in an infinite potential well results in quantized energy levels given by $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$. The normalized eigenfunctions are $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$. This quantization arises due to the boundary conditions imposed by the infinite potential, demonstrating the wave-like nature of particles in confined systems. Such quantization is fundamental to understanding atomic and molecular structures.

25 Normalize the wave function $\psi(x) = e^{-|x|} \sin(ax)$.

Introduction: Normalization of a wave function ensures that the total probability of finding the particle within the entire space is 1. This process involves calculating the normalization constant such that the integral of the probability density over all space equals 1.

Solution:

The given wave function is:

$$\psi(x) = e^{-|x|} \sin(ax)$$

To normalize $\psi(x)$, we must ensure that:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

Calculate $|\psi(x)|^2$:

$$|\psi(x)|^2 = \left(e^{-|x|} \sin(ax) \right)^2 = e^{-2|x|} \sin^2(ax)$$

Now, integrate $|\psi(x)|^2$ over all space:

$$\int_{-\infty}^{\infty} e^{-2|x|} \sin^2(ax) dx$$

Since $e^{-2|x|}$ is an even function and $\sin^2(ax)$ is an even function, the integrand is even. Therefore, we can write:

$$\int_{-\infty}^{\infty} e^{-2|x|} \sin^2(ax) dx = 2 \int_0^{\infty} e^{-2x} \sin^2(ax) dx$$

Using the identity $\sin^2(ax) = \frac{1 - \cos(2ax)}{2}$, the integral becomes:

$$2 \int_0^{\infty} e^{-2x} \frac{1 - \cos(2ax)}{2} dx = \int_0^{\infty} e^{-2x} dx - \int_0^{\infty} e^{-2x} \cos(2ax) dx$$

First, solve $\int_0^{\infty} e^{-2x} dx$:

$$\int_0^{\infty} e^{-2x} dx = \left[\frac{e^{-2x}}{-2} \right]_0^{\infty} = \frac{1}{2}$$

Next, solve $\int_0^{\infty} e^{-2x} \cos(2ax) dx$ using the integral formula for exponential and trigonometric functions:

$$\int_0^{\infty} e^{-bx} \cos(cx) dx = \frac{b}{b^2 + c^2}$$

Here, $b = 2$ and $c = 2a$:

$$\int_0^\infty e^{-2x} \cos(2ax) dx = \frac{2}{4 + 4a^2} = \frac{2}{4(1 + a^2)} = \frac{1}{2(1 + a^2)}$$

Substitute these results back into the integral:

$$\int_{-\infty}^\infty e^{-2|x|} \sin^2(ax) dx = 2 \left(\frac{1}{2} - \frac{1}{2(1 + a^2)} \right) = 1 - \frac{1}{1 + a^2} = \frac{a^2}{1 + a^2}$$

To normalize $\psi(x)$, multiply by the normalization constant N such that:

$$\int_{-\infty}^\infty |N\psi(x)|^2 dx = 1$$

Thus,

$$|N|^2 \int_{-\infty}^\infty e^{-2|x|} \sin^2(ax) dx = 1$$

$$|N|^2 \frac{a^2}{1 + a^2} = 1$$

$$|N|^2 = \frac{1 + a^2}{a^2}$$

$$N = \sqrt{\frac{1 + a^2}{a^2}} = \frac{\sqrt{1 + a^2}}{a}$$

Therefore, the normalized wave function is:

$$\psi(x) = \frac{\sqrt{1 + a^2}}{a} e^{-|x|} \sin(ax)$$

Conclusion: The normalized wave function $\psi(x) = e^{-|x|} \sin(ax)$ is $\psi(x) = \frac{\sqrt{1+a^2}}{a} e^{-|x|} \sin(ax)$. Normalization ensures that the total probability of finding the particle within the entire space is 1, which is a fundamental requirement in quantum mechanics.

26 Consider the one-dimensional wavefunction $\psi(x) = Axe^{-kx}$, ($0 \leq x < \infty$; $k > 0$)

i. Calculate A so that $\psi(x)$ is normalized.

ii. Using Schrödinger's equation find the potential $V(x)$ and energy E for which $\psi(x)$ is an eigenfunction. (Assume that as $x \rightarrow \infty$, $V(x) \rightarrow 0$).

Introduction: The given wavefunction $\psi(x) = Axe^{-kx}$ needs to be normalized and used to find the potential $V(x)$ and energy E for which $\psi(x)$ is an eigenfunction using the Schrödinger equation.

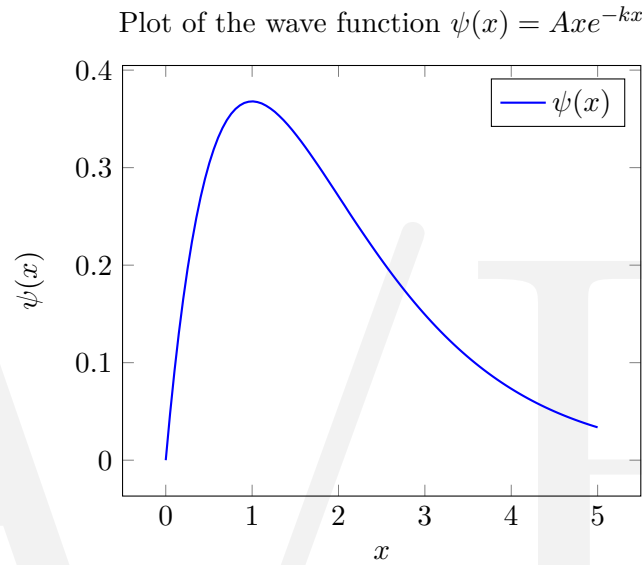


Figure 3: Plot of the wave function $\psi(x) = Axe^{-kx}$

Solution:

i. Calculate A so that $\psi(x)$ is normalized.

To normalize $\psi(x)$, we require:

$$\int_0^{\infty} |\psi(x)|^2 dx = 1$$

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

$$|\psi(x)|^2 = (Axe^{-kx})^2 = A^2 x^2 e^{-2kx}$$

Now, integrate and set it equal to 1:

$$\int_0^{\infty} A^2 x^2 e^{-2kx} dx = 1$$

Using the integral:

$$\int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad a > 0$$

For $n = 2$ and $a = 2k$:

$$\int_0^{\infty} x^2 e^{-2kx} dx = \frac{2!}{(2k)^3} = \frac{2}{8k^3} = \frac{1}{4k^3}$$

Therefore:

$$A^2 \cdot \frac{1}{4k^3} = 1$$

Solving for A :

$$A^2 = 4k^3$$

$$A = 2k^{3/2}$$

ii. Using Schrödinger's equation find the potential $V(x)$ and energy E for which $\psi(x)$ is an eigenfunction. (Assume that as $x \rightarrow \infty$, $V(x) \rightarrow 0$).

The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

First, compute the first and second derivatives of $\psi(x)$:

$$\psi(x) = 2k^{3/2}xe^{-kx}$$

$$\frac{d\psi}{dx} = 2k^{3/2} \left(e^{-kx} - kxe^{-kx} \right) = 2k^{3/2}e^{-kx}(1 - kx)$$

$$\frac{d^2\psi}{dx^2} = 2k^{3/2} \left(-ke^{-kx}(1 - kx) - ke^{-kx} \right) = 2k^{3/2}e^{-kx}(k^2x - 2k)$$

Substitute ψ and its second derivative into the Schrödinger equation:

$$-\frac{\hbar^2}{2m} 2k^{3/2}e^{-kx}(k^2x - 2k) + V(x)2k^{3/2}xe^{-kx} = E2k^{3/2}xe^{-kx}$$

Simplify:

$$-\frac{\hbar^2}{2m} 2k^{3/2}e^{-kx}k(kx - 2) + V(x)2k^{3/2}xe^{-kx} = E2k^{3/2}xe^{-kx}$$

$$-\frac{\hbar^2 k^{5/2}}{m} e^{-kx} \left(x - \frac{2}{k} \right) + V(x)2k^{3/2}xe^{-kx} = E2k^{3/2}xe^{-kx}$$

Divide through by $2k^{3/2}e^{-kx}$:

$$-\frac{\hbar^2 k^2}{2m} \left(x - \frac{2}{k} \right) + V(x)x = Ex$$

Since this must hold for all x :

$$V(x)x = Ex + \frac{\hbar^2 k^2}{2m}x - \frac{\hbar^2 k^2}{m}$$

$$V(x)x = x \left(E + \frac{\hbar^2 k^2}{2m} \right) - \frac{\hbar^2 k^2}{m}$$

Now, solve for $V(x)$:

$$V(x) = E + \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k^2}{mx}$$

Given that as $x \rightarrow \infty$, $V(x) \rightarrow 0$: To satisfy this condition, the constant term in $V(x)$ must be zero:

$$E + \frac{\hbar^2 k^2}{2m} = 0$$

This gives us:

$$E = -\frac{\hbar^2 k^2}{2m}$$

Therefore, the potential $V(x)$ becomes:

$$V(x) = -\frac{\hbar^2 k^2}{m} \left(\frac{1}{x} \right)$$

Conclusion: The normalization constant A is found to be $2k^{3/2}$. Using the Schrödinger equation, the potential $V(x)$ and energy E for which $\psi(x)$ is an eigenfunction are determined. The energy is $E = -\frac{\hbar^2 k^2}{2m}$ and the potential is $V(x) = -\frac{\hbar^2 k^2}{m} \left(\frac{1}{x} \right)$.

A/P

- 27 (a) Solve the radial part of the time-independent Schrödinger equation for a hydrogen atom. Obtain an expression for the energy eigenvalues.
 (b) What is the degree of degeneracy of the energy eigenvalues? What happens if the spin of the electron is taken into account?

(a) **Introduction:** The hydrogen atom problem is a classic problem in quantum mechanics. It involves solving the Schrödinger equation for an electron bound to a proton via the Coulomb potential. The solution provides the allowed energy levels of the electron, explaining the discrete spectral lines of hydrogen.

Solution:

The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi$$

For the hydrogen atom, the potential $V(r)$ is the Coulomb potential:

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

We separate the wavefunction ψ into radial and angular parts:

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$$

The Laplacian in spherical coordinates is given by:

$$\begin{aligned}\nabla^2\psi = & \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)Y(\theta, \phi) \\ & + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y(\theta, \phi)}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 Y(\theta, \phi)}{\partial\phi^2}\end{aligned}$$

Substituting this into the Schrödinger equation:

$$\begin{aligned}-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)Y(\theta, \phi) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y(\theta, \phi)}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 Y(\theta, \phi)}{\partial\phi^2}\right] \\ - \frac{e^2}{4\pi\epsilon_0 r}R(r)Y(\theta, \phi) = ER(r)Y(\theta, \phi)\end{aligned}$$

Divide through by $R(r)Y(\theta, \phi)$:

$$\begin{aligned}-\frac{\hbar^2}{2m}\left[\frac{1}{R(r)}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) + \frac{1}{Y(\theta, \phi)}\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y(\theta, \phi)}{\partial\theta}\right) + \frac{1}{Y(\theta, \phi)}\frac{1}{r^2\sin^2\theta}\frac{\partial^2 Y(\theta, \phi)}{\partial\phi^2}\right] \\ - \frac{e^2}{4\pi\epsilon_0 r} = E\end{aligned}$$

Multiply through by $2m$ and r^2 to separate variables:

$$\begin{aligned} & \left[-\frac{\hbar^2}{2m} \frac{1}{R(r)} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) - \frac{e^2 r^2}{4\pi\epsilon_0 \hbar^2} \right] \\ &= \left[\frac{1}{Y(\theta, \phi) \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{Y(\theta, \phi) \sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} \right] = -\frac{2mEr^2}{\hbar^2} \end{aligned}$$

Since the left side is a function of r only and the right side is a function of θ and ϕ only, both sides must be equal to a constant, which we denote as $l(l+1)$:

For the radial part:

$$-\frac{\hbar^2}{2m} \frac{1}{R(r)} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) - \frac{e^2 r^2}{4\pi\epsilon_0 \hbar^2} = l(l+1)$$

Rewriting and simplifying:

$$\frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \left[\frac{2m}{\hbar^2} \left(E + \frac{e^2}{4\pi\epsilon_0 r} \right) r^2 - l(l+1) \right] R(r) = 0$$

Introducing the substitution:

$$R(r) = \frac{u(r)}{r}$$

We obtain:

$$\frac{d^2 u(r)}{dr^2} + \left[\frac{2m}{\hbar^2} \left(E + \frac{e^2}{4\pi\epsilon_0 r} \right) - \frac{l(l+1)}{r^2} \right] u(r) = 0$$

To solve this equation, we introduce dimensionless variables:

$$\rho = \frac{r}{a_0}, \quad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2}$$

and let

$$\epsilon = \frac{Ea_0}{e^2/4\pi\epsilon_0}$$

Substituting these into the radial equation, we get:

$$\frac{d^2 u(\rho)}{d\rho^2} + \left[-\frac{1}{\rho} + \frac{l(l+1)}{\rho^2} - \epsilon \right] u(\rho) = 0$$

This is a standard equation. Thus, the energy eigenvalues are given by:

$$E_n = -\frac{me^4}{2\hbar^2(4\pi\epsilon_0)^2} \frac{1}{n^2}$$

where n is the principal quantum number.

Conclusion: The radial part of the Schrödinger equation for the hydrogen atom yields energy eigenvalues given by $E_n = -\frac{me^4}{2\hbar^2(4\pi\epsilon_0)^2} \frac{1}{n^2}$. These eigenvalues explain the discrete energy levels observed in the hydrogen atom spectrum.

(b) **Introduction:** The energy levels of the hydrogen atom have a certain degree of degeneracy due to the multiple quantum states that share the same energy.

Solution:

The degree of degeneracy of the energy eigenvalues for a given principal quantum number n is:

$$\sum_{l=0}^{n-1} (2l+1) = n^2$$

This sum accounts for all possible values of the angular momentum quantum number l and its corresponding magnetic quantum number m .

When the spin of the electron is taken into account, each spatial state can have two possible spin states (spin-up and spin-down). Thus, the degeneracy is doubled:

$$2n^2$$

Conclusion: The degree of degeneracy of the energy eigenvalues for the hydrogen atom is n^2 . When electron spin is considered, this degeneracy increases to $2n^2$, reflecting the two possible spin states for each spatial quantum state.

A/P

28 Obtain the time-dependent Schrödinger equation for a particle. Hence deduce the time-independent Schrödinger equation.

Introduction:

The Schrödinger equation is fundamental to quantum mechanics, describing how the quantum state of a physical system changes over time. This derivation starts from basic principles, using the classical wave equation analogy and the principle of energy conservation, to derive both the time-dependent and time-independent Schrödinger equations.

Solution:

1. Derivation of the Time-Dependent Schrödinger Equation

We start with the classical wave equation for a free particle in one dimension. The classical wave equation is given by:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}$$

In quantum mechanics, the wavefunction ψ represents the probability amplitude, and we need to incorporate the energy of the particle into the wave equation. The total energy E of a particle is given by the sum of its kinetic and potential energies:

$$E = T + V$$

For a free particle (where the potential $V = 0$), the kinetic energy T is given by:

$$T = \frac{p^2}{2m}$$

where p is the momentum of the particle. In quantum mechanics, the momentum operator $\hat{p}$ is given by:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

Thus, the kinetic energy operator $\hat{T}$ becomes:

$$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

The total energy operator $\hat{E}$ acting on the wavefunction ψ gives:

$$\hat{E}\psi = E\psi = i\hbar \frac{\partial \psi}{\partial t}$$

Combining these, we get the time-dependent Schrödinger equation for a free particle:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

When a potential $V(x, t)$ is present, the Schrödinger equation generalizes to:

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x, t)\psi \right)$$

This is the time-dependent Schrödinger equation.

2. Derivation of the Time-Independent Schrödinger Equation

To derive the time-independent Schrödinger equation, we assume the potential $V(x, t) = V(x)$ is time-independent, and seek solutions of the form:

$$\psi(x, t) = \phi(x)T(t)$$

Substituting this into the time-dependent Schrödinger equation, we get:

$$i\hbar \left(\phi(x) \frac{dT(t)}{dt} \right) = \left(-\frac{\hbar^2}{2m} \frac{d^2 \phi(x)}{dx^2} + V(x)\phi(x) \right) T(t)$$

Dividing both sides by $\phi(x)T(t)$, we obtain:

$$i\hbar \frac{1}{T(t)} \frac{dT(t)}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\phi(x)} \frac{d^2 \phi(x)}{dx^2} + V(x)$$

Since the left-hand side is a function of time only and the right-hand side is a function of space only, both sides must be equal to a constant, which we denote by E . This gives us two separate equations:

For the time part:

$$i\hbar \frac{dT(t)}{dt} = ET(t)$$

Solving this differential equation, we get:

$$T(t) = e^{-iEt/\hbar}$$

For the spatial part, we get the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 \phi(x)}{dx^2} + V(x)\phi(x) = E\phi(x)$$

Conclusion:

We have derived the time-dependent Schrödinger equation, which describes the evolution of a quantum state over time. By assuming a separable solution and a time-independent potential, we derived the time-independent Schrödinger equation, which is used to find the stationary states of a quantum system. These equations are fundamental to quantum mechanics and are essential for understanding the behavior of quantum systems.

29 Solve the Schrödinger equation for a particle of mass m confined in a one-dimensional potential well of the form

$$V(x) = \begin{cases} 0 & ; 0 \leq x \leq L \\ \infty & ; x < 0, x > L \end{cases}$$

Obtain the discrete energy values and the normalized eigenfunctions.

Introduction: The problem of a particle in a one-dimensional potential well (also known as an infinite potential well or "particle in a box") is a fundamental quantum mechanics problem. It provides insight into the quantization of energy levels and the behavior of particles in confined spaces.

Solution:

Solving to find the Schrödinger Equation in the Potential Well:

The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

For the potential well defined by:

$$V(x) = \begin{cases} 0 & ; 0 \leq x \leq L \\ \infty & ; x < 0, x > L \end{cases}$$

Within the well ($0 \leq x \leq L$), the potential $V(x) = 0$, so the Schrödinger equation simplifies to:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

Rearranging, we get:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

Let:

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

The equation becomes:

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

The general solution to this differential equation is:

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

Checking for Boundary Conditions:

The boundary conditions are:

$$\psi(0) = 0 \quad \text{and} \quad \psi(L) = 0$$

Applying the boundary condition at $x = 0$:

$$\psi(0) = A \sin(0) + B \cos(0) = B = 0$$

Thus, the wave-function simplifies to:

$$\psi(x) = A \sin(kx)$$

Applying the boundary condition at $x = L$:

$$\psi(L) = A \sin(kL) = 0$$

For this equation to hold, $\sin(kL)$ must be zero, which implies:

$$kL = n\pi \quad \text{where} \quad n = 1, 2, 3, \dots$$

Thus:

$$k = \frac{n\pi}{L}$$

Finding the Discrete Energy Values:

Substituting k back into the expression for energy E :

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L} \right)^2 = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

So, the discrete energy levels are:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{where} \quad n = 1, 2, 3, \dots$$

Constructing Normalized Eigen-functions:

The wavefunction is given by:

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

To normalize $\psi_n(x)$, we require:

$$\int_0^L |\psi_n(x)|^2 dx = 1$$

Substituting $\psi_n(x)$:

$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

Using the integral:

$$\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}$$

We get:

$$A^2 \cdot \frac{L}{2} = 1 \quad \Rightarrow \quad A^2 = \frac{2}{L} \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}$$

Thus, the normalized eigen-functions are:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Conclusion: For a particle in a one-dimensional infinite potential well, the energy levels are quantized and given by $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$. The corresponding normalized eigen-functions are $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$, showing the wave nature of particles in a confined space.

30 An electron is moving in a one-dimensional box of infinite height and width 1 Å. Find the minimum energy of electron.

Introduction: In quantum mechanics, a particle confined in a one-dimensional box (infinite potential well) exhibits quantized energy levels. The minimum energy corresponds to the ground state.

Solution:

For an electron in a one-dimensional box of width $L = 1 \text{ Å} = 1 \times 10^{-10} \text{ m}$, the energy levels are given by:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

The minimum energy corresponds to the ground state ($n = 1$):

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

Substitute the values: - Planck's constant $\hbar = 1.0545718 \times 10^{-34} \text{ J} \cdot \text{s}$ - Electron mass $m = 9.10938356 \times 10^{-31} \text{ kg}$ - Width $L = 1 \times 10^{-10} \text{ m}$

Calculating:

$$E_1 = \frac{\pi^2(1.0545718 \times 10^{-34})^2}{2(9.10938356 \times 10^{-31})(1 \times 10^{-10})^2}$$

$$E_1 \approx 6.024 \times 10^{-18} \text{ J}$$

To convert this energy into electronvolts (eV):

$$1 \text{ eV} = 1.60218 \times 10^{-19} \text{ J}$$

$$E_1 \approx \frac{6.024 \times 10^{-18}}{1.60218 \times 10^{-19}} \text{ eV}$$

$$E_1 \approx 37.6 \text{ eV}$$

Conclusion: The minimum energy of an electron confined in a one-dimensional box of width 1 Å is approximately 37.6 eV.

31 Normalized wave function of a particle is given:

$$\psi(x) = N \exp \left(-\frac{x^2}{2a^2} + ikx \right).$$

Find the expectation value of position.

Introduction:

The expectation value of position $\langle x \rangle$ for a given wavefunction $\psi(x)$ is defined as:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx,$$

where $|\psi(x)|^2 = \psi^*(x)\psi(x)$ represents the probability density of the particle.

Solution:

Given:

$$\psi(x) = N \exp \left(-\frac{x^2}{2a^2} + ikx \right),$$

its complex conjugate is:

$$\psi^*(x) = N^* \exp \left(-\frac{x^2}{2a^2} - ikx \right).$$

Then the probability density becomes:

$$|\psi(x)|^2 = \psi^*(x)\psi(x) = |N|^2 \exp \left(-\frac{x^2}{a^2} \right).$$

Note that $\left| \exp \left(-\frac{x^2}{2a^2} \right) \right|^2 = \exp \left(-\frac{x^2}{a^2} \right)$ since the argument is real, and $|e^{ikx}|^2 = 1$ since k is real. Therefore:

Now compute the expectation value:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = |N|^2 \int_{-\infty}^{\infty} x \exp \left(-\frac{x^2}{a^2} \right) dx.$$

Note that $x \exp \left(-\frac{x^2}{a^2} \right)$ is an odd function, and the limits of integration are symmetric about zero. Therefore,

$$\langle x \rangle = 0.$$

Conclusion:

The expectation value of the position for the given wavefunction is zero. This result reflects the symmetry of the probability distribution, which is centered about the origin, indicating that the average position of the particle is at $x = 0$.

32 Write the time-independent Schrödinger equation for a bouncing ball.

Introduction:

In quantum mechanics, a bouncing ball can be modeled as a particle subject to a gravitational potential. The potential energy increases linearly with height, similar to the classical potential energy function in a gravitational field.

Solution:

For a bouncing ball, the potential energy $V(z)$ is given by:

$$V(z) = mgz$$

where: - m is the mass of the ball, - g is the acceleration due to gravity, - z is the height above the ground.

The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(z)}{dz^2} + V(z)\psi(z) = E\psi(z)$$

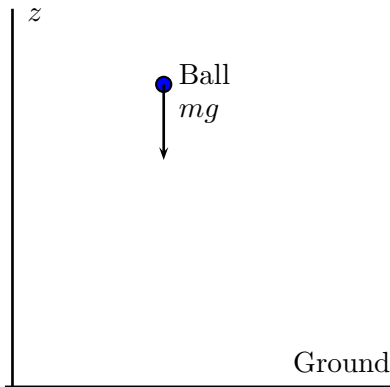
Substituting the potential $V(z) = mgz$, we get:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(z)}{dz^2} + mgz\psi(z) = E\psi(z)$$

Rewriting, we have:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(z)}{dz^2} + mgz\psi(z) = E\psi(z)$$

This is the time-independent Schrödinger equation for a particle in a linear potential, representing a bouncing ball in a gravitational field.



Conclusion:

The time-independent Schrödinger equation for a bouncing ball subject to a gravitational potential is given by:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(z)}{dz^2} + mgz\psi(z) = E\psi(z)$$

This equation models the quantum behavior of a particle under the influence of gravity, providing insight into the quantized energy levels and wavefunctions of a bouncing ball in a gravitational field.

33 Solve the Schrödinger equation for a step potential and calculate the transmission and reflection coefficients for the case when the kinetic energy of the particle E_0 is greater than the potential energy V (i.e., $E_0 > V$).

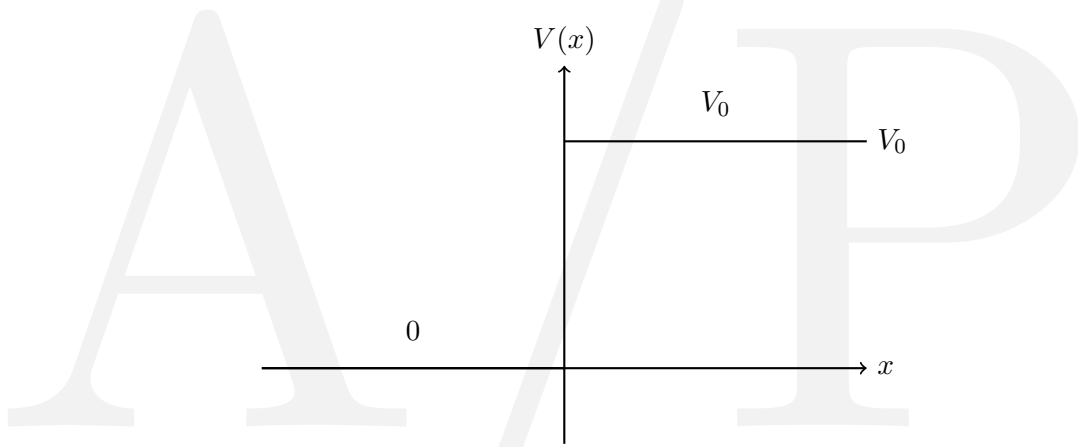
Introduction:

The step potential is a fundamental problem in quantum mechanics that illustrates the behavior of a particle encountering a sudden change in potential energy. This problem is essential for understanding phenomena such as quantum tunneling and reflection.

Consider a particle encountering a step potential:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x \geq 0 \end{cases}$$

Below is a diagram illustrating the step potential:



Solution:

Consider a particle encountering a step potential:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x \geq 0 \end{cases}$$

The Schrödinger equation in regions where $V(x)$ is constant is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

For $x < 0$ (Region I), where $V(x) = 0$:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E_0\psi(x)$$

The general solution is:

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

where:

$$k_1 = \sqrt{\frac{2mE_0}{\hbar^2}}$$

For $x \geq 0$ (Region II), where $V(x) = V_0$:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E_0\psi(x)$$

This simplifies to:

$$\frac{d^2\psi(x)}{dx^2} = k_2^2\psi(x)$$

where:

$$k_2 = \sqrt{\frac{2m(E_0 - V_0)}{\hbar^2}}$$

The general solution is:

$$\psi_{II}(x) = Ce^{ik_2x}$$

Since we consider the particle coming from the left and moving to the right, there will be no wave traveling to the left in Region II ($D = 0$):

$$\psi_{II}(x) = Ce^{ik_2x}$$

Boundary Conditions:

At $x = 0$, the wavefunctions and their first derivatives must be continuous:

$$\begin{aligned}\psi_I(0) &= \psi_{II}(0) \\ \left. \frac{d\psi_I}{dx} \right|_{x=0} &= \left. \frac{d\psi_{II}}{dx} \right|_{x=0}\end{aligned}$$

Applying these conditions:

1. Continuity of wavefunction:

$$A + B = C$$

2. Continuity of derivative:

$$ik_1A - ik_1B = ik_2C$$

Solving these equations for A , B , and C :

From the first equation:

$$C = A + B$$

Substituting into the second equation:

$$ik_1A - ik_1B = ik_2(A + B)$$

Rearranging:

$$k_1A - k_1B = k_2A + k_2B$$

$$(k_1 - k_2)A = (k_1 + k_2)B$$

$$\frac{A}{B} = \frac{k_1 + k_2}{k_1 - k_2}$$

Therefore, the reflection coefficient R is:

$$R = \left| \frac{B}{A} \right|^2 = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2$$

The transmission coefficient T is given by:

$$T = \left| \frac{C}{A} \right|^2 = \left| \frac{2k_1}{k_1 + k_2} \right|^2$$

Conclusion:

For a particle encountering a step potential with $E_0 > V_0$, the transmission and reflection coefficients are given by:

$$R = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2, \quad T = \left| \frac{2k_1}{k_1 + k_2} \right|^2$$

These coefficients describe the probability of the particle being reflected or transmitted at the potential step.

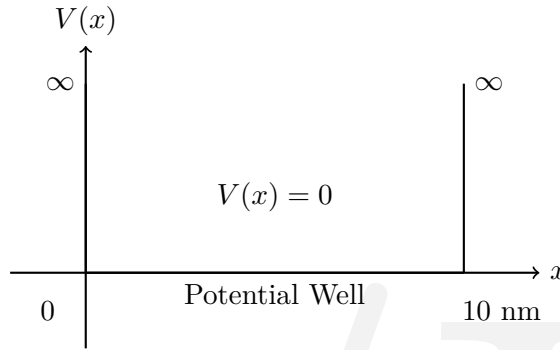
An application of the step potential is seen in the behavior of electrons in semiconductor devices, where they encounter potential barriers at junctions, leading to phenomena like tunneling and reflection that are crucial for the operation of diodes and transistors.

34 Calculate the lowest energy of an electron confined to move in a 1-dimensional potential well of width 10 nm.

Introduction:

The problem of an electron confined in a one-dimensional potential well, also known as a "particle in a box," demonstrates the concept of quantized energy levels in quantum mechanics.

Below is a diagram illustrating the one-dimensional potential well:



Solution:

For an electron in a one-dimensional box of width $L = 10 \text{ nm} = 10 \times 10^{-9} \text{ m}$, the energy levels are given by:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

The normalized wave function is:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

The lowest energy corresponds to the ground state ($n = 1$):

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

Substitute the values: - Planck's constant $\hbar = 1.0545718 \times 10^{-34} \text{ J} \cdot \text{s}$ - Electron mass $m = 9.10938356 \times 10^{-31} \text{ kg}$ - Width $L = 10 \times 10^{-9} \text{ m}$

Calculating:

$$E_1 = \frac{\pi^2 (1.0545718 \times 10^{-34})^2}{2(9.10938356 \times 10^{-31})(10 \times 10^{-9})^2}$$

$$E_1 \approx 6.024 \times 10^{-20} \text{ J}$$

To convert this energy into electronvolts (eV):

$$1 \text{ eV} = 1.60218 \times 10^{-19} \text{ J}$$

$$E_1 \approx \frac{6.024 \times 10^{-20}}{1.60218 \times 10^{-19}} \text{ eV}$$

$$E_1 \approx 0.376 \text{ eV}$$

Conclusion:

The lowest energy of an electron confined in a one-dimensional potential well of width 10 nm is approximately 0.376 eV.

A/P

35 Using Schrödinger Equation to Obtain Eigen-functions and Eigenvalues for a 1-Dimensional Harmonic Oscillator. Sketch the profiles of eigenfunctions for first three energy states.

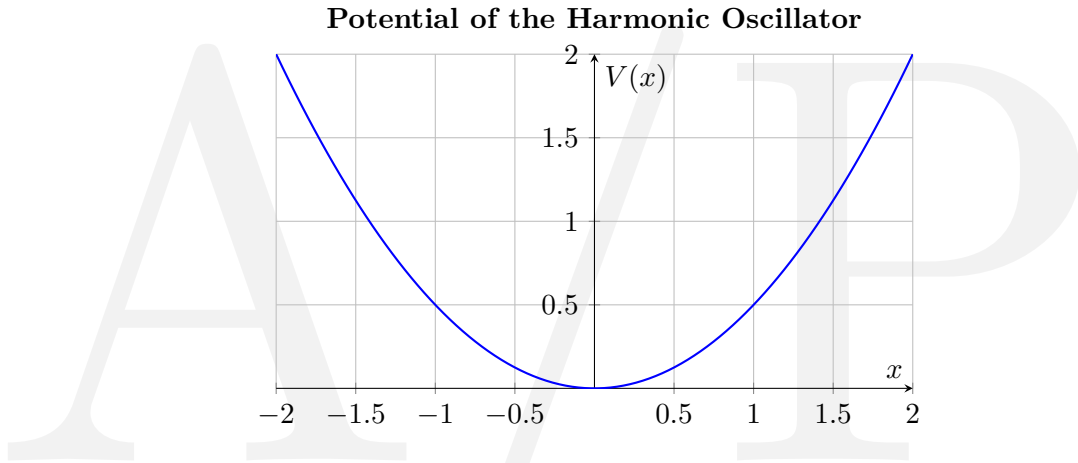
Introduction:

The quantum harmonic oscillator is a fundamental model in quantum mechanics that describes a particle subject to a restoring force proportional to its displacement from equilibrium. This is represented by the potential energy function:

$$V(x) = \frac{1}{2}m\omega^2x^2$$

where m is the mass of the particle and ω is the angular frequency of the oscillator. This potential is quadratic in x , making it an ideal system to illustrate quantized energy levels and wavefunctions.

Below is a graph illustrating the potential $V(x)$ of a harmonic oscillator:



Solution:

The force acting on a particle executing linear harmonic oscillation is given by Hooke's law:

$$F = -kx$$

where x represents the displacement from the equilibrium position, and k is the force constant. This linear relationship indicates that the force is always directed towards the equilibrium position and its magnitude increases linearly with the displacement.

The corresponding potential energy function, $V(x)$, associated with this force is quadratic and is expressed as:

$$V(x) = \frac{1}{2}kx^2$$

In terms of the mass m of the particle and the angular frequency ω , where $\omega = \sqrt{\frac{k}{m}}$, the potential energy can be rewritten as:

$$V(x) = \frac{1}{2}m\omega^2x^2$$

The time-independent Schrödinger equation for a particle of mass m in this potential is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x)$$

Simplifying, we obtain:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} \left(E - \frac{1}{2}m\omega^2 x^2 \right) \psi(x) = 0$$

To simplify this equation, we introduce the dimensionless eigenvalue λ and the dimensionless variable ξ :

$$\lambda = \frac{2E}{\hbar\omega}$$

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x$$

Substituting these into the Schrödinger equation transforms it into:

$$\frac{d^2\psi(\xi)}{d\xi^2} + (\lambda - \xi^2) \psi(\xi) = 0$$

This differential equation is known as the Hermite equation. The solutions to this equation are the Hermite polynomials $H_n(\xi)$. The eigenfunctions of the harmonic oscillator are thus given by:

$$\psi_n(\xi) = A_n H_n(\xi) e^{-\xi^2/2}$$

where A_n is the normalization constant. These polynomials satisfy the orthogonality condition and are well-suited to describe the quantum states of the harmonic oscillator.

To solve the Hermite equation, we assume a power series solution:

$$\psi(\xi) = e^{-\xi^2/2} \sum_{n=0}^{\infty} a_n \xi^n$$

Substituting this series into the differential equation and matching coefficients for each power of ξ , we derive a recurrence relation for the coefficients a_n :

First, we compute the derivatives:

$$\begin{aligned} \frac{d\psi(\xi)}{d\xi} &= e^{-\xi^2/2} \left(\sum_{n=0}^{\infty} a_n n \xi^{n-1} - \xi \sum_{n=0}^{\infty} a_n \xi^n \right) \\ &= e^{-\xi^2/2} \left(\sum_{n=1}^{\infty} a_n n \xi^{n-1} - \xi \sum_{n=0}^{\infty} a_n \xi^n \right) \\ &= e^{-\xi^2/2} \left(\sum_{n=1}^{\infty} a_n n \xi^{n-1} - \sum_{n=0}^{\infty} a_n \xi^{n+1} \right) \end{aligned}$$

Then,

$$\begin{aligned} \frac{d^2\psi(\xi)}{d\xi^2} &= e^{-\xi^2/2} \left(\sum_{n=1}^{\infty} a_n n(n-1) \xi^{n-2} - 2\xi \sum_{n=1}^{\infty} a_n n \xi^{n-1} + \xi^2 \sum_{n=0}^{\infty} a_n \xi^n \right) \\ &= e^{-\xi^2/2} \left(\sum_{n=2}^{\infty} a_n n(n-1) \xi^{n-2} - 2 \sum_{n=1}^{\infty} a_n n \xi^n + \sum_{n=0}^{\infty} a_n \xi^{n+2} \right) \end{aligned}$$

Rewriting the Schrödinger equation:

$$e^{-\xi^2/2} \left(\sum_{n=2}^{\infty} a_n n(n-1) \xi^{n-2} - 2 \sum_{n=1}^{\infty} a_n n \xi^n + \sum_{n=0}^{\infty} a_n \xi^{n+2} \right) + (\lambda - \xi^2) e^{-\xi^2/2} \sum_{n=0}^{\infty} a_n \xi^n = 0$$

Grouping terms by the power of ξ :

$$\sum_{n=2}^{\infty} a_n n(n-1) \xi^{n-2} - 2 \sum_{n=1}^{\infty} a_n n \xi^n + \sum_{n=0}^{\infty} a_n \xi^{n+2} + \lambda \sum_{n=0}^{\infty} a_n \xi^n - \sum_{n=0}^{\infty} a_n \xi^{n+2} = 0$$

$$\sum_{n=0}^{\infty} (a_{n+2}(n+2)(n+1) - 2a_n n + \lambda a_n) \xi^n = 0$$

For the series to terminate, ensuring normalizable wavefunctions, λ must be an odd integer:

$$\lambda = 2n + 1$$

Thus, the quantized energy levels are given by:

$$E_n = \left(n + \frac{1}{2} \right) \hbar \omega$$

The corresponding normalized eigenfunctions are derived as follows:

The power series solution:

$$\psi(\xi) = e^{-\xi^2/2} \sum_{n=0}^{\infty} a_n \xi^n$$

Substituting into the Schrödinger equation:

$$\frac{d^2 \psi(\xi)}{d\xi^2} + (\lambda - \xi^2) \psi(\xi) = 0$$

The Hermite polynomials $H_n(\xi)$ are defined as:

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} \left(e^{-\xi^2} \right)$$

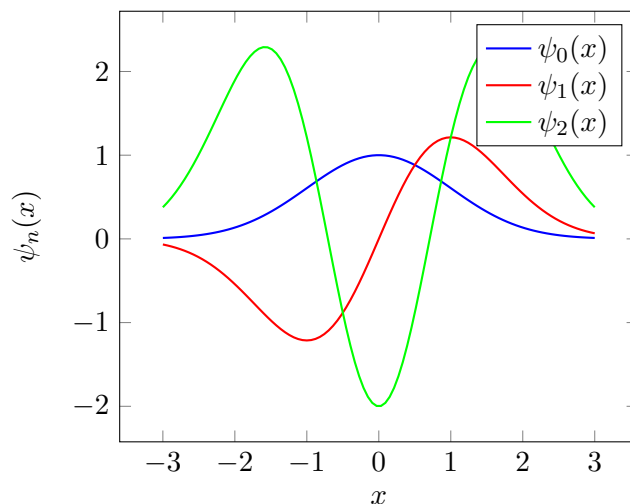
The normalized eigenfunctions are:

$$\psi_n(\xi) = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} H_n(\alpha \xi) e^{-\alpha^2 \xi^2/2}$$

where $\alpha = \sqrt{\frac{m\omega}{\hbar}}$.

Below are the plots of the first three eigenfunctions:

First Three Eigenfunctions of the Harmonic Oscillator



Conclusion

(i) The peculiar point is the ground state wave function of simple harmonic oscillator that is Gaussian in nature. This arises due to the unique boundary conditions of the system. SHO is the only system for which **equality of Heisenberg uncertainty principle** holds true (in ground state).

(ii) The derived **energy eigenvalues** $E_n = (n + \frac{1}{2}) \hbar\omega$ are quantized, meaning the system can only occupy specific energy levels. This indicates discrete energy states rather than a continuum.

(iii) **Applications:** Molecular Vibrations in Chemistry, where it explains the spectra observed in **infrared spectroscopy**. In quantum field theory, it serves as the basis for understanding **particle behavior in potential wells and for modeling quantized fields**.

36 Calculate the probability of transmission of an electron of 1.0 eV energy through a potential barrier of 4.0 eV and 0.1 nm width.

Introduction:. Here Quantum tunneling is taking place. Quantum tunneling occurs when particles pass through a barrier that they classically shouldn't be able to, due to their energy being lower than the potential of the barrier.

Solution:

The transmission probability T for a particle with energy E encountering a potential barrier V of width a is given by:

$$T = \exp(-2\kappa a)$$

where:

$$\kappa = \sqrt{\frac{2m(V - E)}{\hbar^2}}$$

Given:

- Energy $E = 1.0$ eV
- Potential $V = 4.0$ eV
- Width $a = 0.1$ nm $= 0.1 \times 10^{-9}$ m
- Electron mass $m = 9.10938356 \times 10^{-31}$ kg
- Planck's constant $\hbar = 1.0545718 \times 10^{-34}$ J · s
- 1 eV $= 1.60218 \times 10^{-19}$ J

Calculate κ :

$$\kappa = \sqrt{\frac{2 \times 9.10938356 \times 10^{-31} \times (4.0 - 1.0) \times 1.60218 \times 10^{-19}}{(1.0545718 \times 10^{-34})^2}}$$

$$\kappa \approx 1.14 \times 10^{10} \text{ m}^{-1}$$

Calculate the transmission probability:

$$T = \exp(-2 \times 1.14 \times 10^{10} \times 0.1 \times 10^{-9})$$

$$T = \exp(-2 \times 1.14)$$

$$T \approx \exp(-2.28)$$

$$T \approx 0.102$$

Conclusion: The probability of transmission of an electron with 1.0 eV energy through a potential barrier of 4.0 eV and 0.1 nm width is **approximately 0.102**, illustrating the quantum tunneling effect. Quantum tunneling is significant in various applications such as in the operation of **tunnel diodes** and the process of nuclear fusion in stars. This phenomenon also underpins the functionality of **scanning tunneling microscopes**, which can image surfaces at the atomic level.

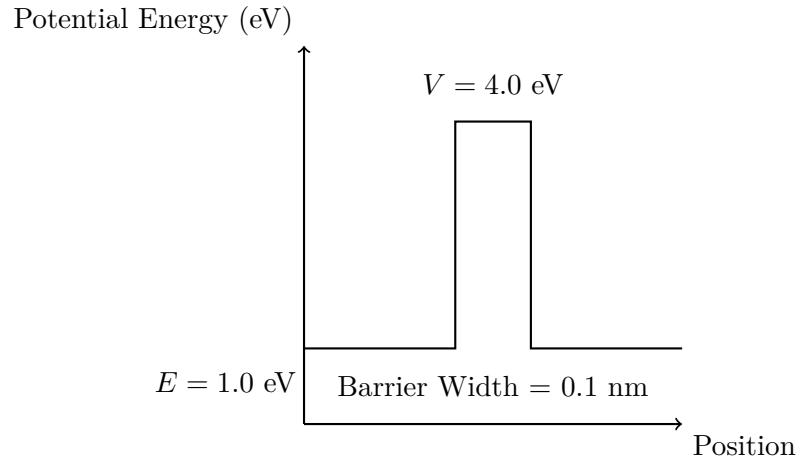
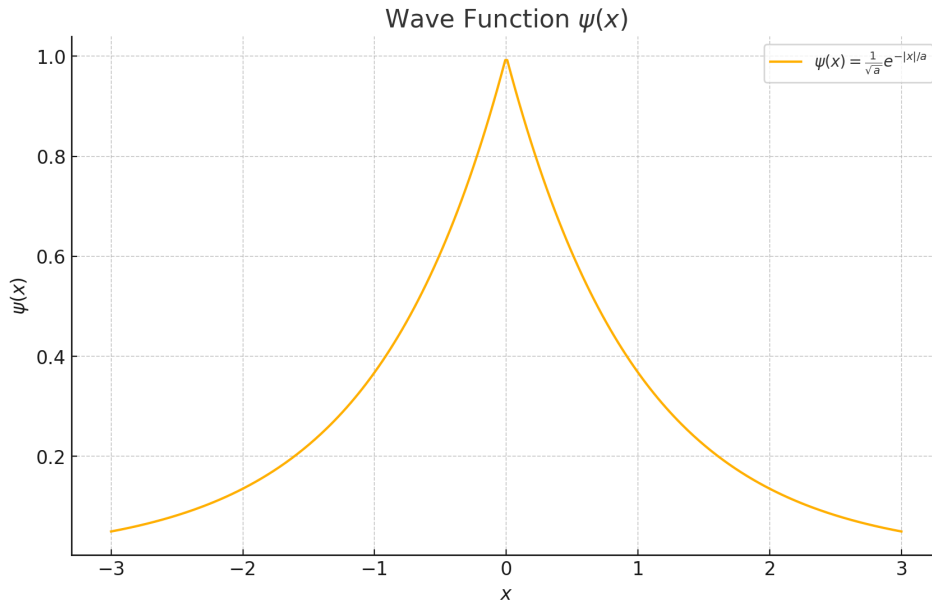


Figure 4: Potential Barrier Diagram

37 The wave function of a particle is given as $\psi(x) = \frac{1}{\sqrt{a}}e^{-|x|/a}$. Find the probability of locating the particle in the range $-a \leq x \leq a$.

Introduction: The wave function $\psi(x)$ provides the probability amplitude for finding a particle at position x . The probability of locating the particle in a specific range is given by the integral of the square of the wave function over that range.



The general expression for the probability P of finding the particle in the range $x_1 \leq x \leq x_2$ is given by:

$$P = \int_{x_1}^{x_2} |\psi(x)|^2 dx$$

Solution: The probability P of finding the particle in the range $-a \leq x \leq a$ is given by:

$$P = \int_{-a}^a |\psi(x)|^2 dx$$

Given the wave function:

$$\psi(x) = \frac{1}{\sqrt{a}} e^{-|x|/a}$$

The square of the wave function is:

$$|\psi(x)|^2 = \left(\frac{1}{\sqrt{a}} e^{-|x|/a} \right)^2 = \frac{1}{a} e^{-2|x|/a}$$

Thus, the probability is:

$$P = \int_{-a}^a \frac{1}{a} e^{-2|x|/a} dx$$

Since the wave function is symmetric about $x = 0$, we can simplify the integral:

$$P = 2 \int_0^a \frac{1}{a} e^{-2x/a} dx$$

Evaluating the integral:

$$\begin{aligned} P &= 2 \left[-\frac{1}{2} e^{-2x/a} \right]_0^a \\ P &= 2 \left[-\frac{1}{2} e^{-2a/a} + \frac{1}{2} \right] \\ P &= 2 \left[-\frac{1}{2} e^{-2} + \frac{1}{2} \right] \\ P &= 1 - e^{-2} \end{aligned}$$

Conclusion: The probability of locating the particle in the range $-a \leq x \leq a$ is $1 - e^{-2}$. This result illustrates how the wave function's exponential decay affects the probability distribution within a finite range.

38 Calculate the zero-point energy of a system consisting of a mass of 10^{-3} kg connected to a fixed point by a spring which is stretched by 10^{-2} m by a force of 10^{-1} N. The system is constrained to move only in one direction.

Introduction:

Zero-point energy is the lowest possible energy that a quantum mechanical physical system may have. It is the energy of the ground state of the system. In the case of a harmonic oscillator, the zero-point energy is $\frac{1}{2}\hbar\omega$, where ω is the angular frequency of the oscillator.

Solution:

First, we need to determine the spring constant k using Hooke's Law:

$$F = kx$$

Given:

- Force, $F = 10^{-1}$ N
- Displacement, $x = 10^{-2}$ m

We solve for k :

$$k = \frac{F}{x} = \frac{10^{-1}}{10^{-2}} = 10 \text{ N/m}$$

Next, we find the angular frequency ω of the system:

$$\omega = \sqrt{\frac{k}{m}}$$

Given:

- Mass, $m = 10^{-3}$ kg
- Spring constant, $k = 10$ N/m

We solve for ω :

$$\omega = \sqrt{\frac{10}{10^{-3}}} = \sqrt{10^4} = 100 \text{ rad/s}$$

The zero-point energy E_0 of a quantum harmonic oscillator is given by:

$$E_0 = \frac{1}{2}\hbar\omega$$

Using the reduced Planck constant $\hbar \approx 1.054 \times 10^{-34}$ Js, we get:

$$E_0 = \frac{1}{2} \times 1.054 \times 10^{-34} \times 100 = 5.27 \times 10^{-33} \text{ J}$$

Conclusion:

The zero-point energy of the system is 5.27×10^{-33} J. This energy represents the lowest energy state of the harmonic oscillator system, even at absolute zero temperature. This concept illustrates the inherent energy present in all quantum systems due to the Heisenberg uncertainty principle.

39 The general wave function of harmonic oscillator (one-dimensional) are of the form

$$u_n(x) = \sum_{k=0}^{\infty} a_k y^k e^{-y^2/2}$$

with $y = \sqrt{\frac{m\omega}{\hbar}}x$, and coefficients a_k are determined by recurrence relations

$$a_{k+2} = \frac{2(k-n)}{(k+1)(k+2)} a_k$$

Corresponding energy levels are

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

Discuss the parity of these wave functions. What happens, if the potential for $x \leq 0$ is infinite (half harmonic oscillator)?

Introduction:

The general wave function of a one-dimensional harmonic oscillator is given by a series solution involving Hermite polynomials. The parity of a wave function refers to its behavior under spatial inversion, $x \rightarrow -x$.

Solution:

1. Wave Function and Recurrence Relation:

The wave function $u_n(x)$ is expressed as a series involving the Hermite polynomials $H_n(y)$:

$$u_n(x) = H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{m\omega x^2}{2\hbar}}$$

The coefficients a_k in the series are determined by the recurrence relation:

$$a_{k+2} = \frac{2(k-n)}{(k+1)(k+2)} a_k$$

2. Parity of Wave Functions:

The wave functions $u_n(x)$ for the harmonic oscillator have definite parity:

$$u_n(-x) = (-1)^n u_n(x)$$

This means:

- For even n : $u_n(x)$ is an even function.
- For odd n : $u_n(x)$ is an odd function.

This behavior is a result of the properties of the Hermite polynomials, which alternate in parity.

3. Half Harmonic Oscillator:

If the potential is infinite for $x \leq 0$, the wave function must vanish at $x = 0$:

$$u_n(0) = 0$$

For the half harmonic oscillator, this condition is satisfied only by the odd-parity solutions:

- Only wave functions with odd n are valid.
- These wave functions naturally vanish at $x = 0$, satisfying the boundary condition.

Conclusion:

The wave functions of a harmonic oscillator exhibit definite parity, with even n corresponding to even functions and odd n corresponding to odd functions. For a half harmonic oscillator, where the potential is infinite for $x \leq 0$, only the odd-parity wave functions are valid, as they meet the boundary condition $u_n(0) = 0$. This restriction reduces the number of allowed energy levels and changes the overall behavior of the system.

A/P

40 Which of the following functions is/are acceptable solution(s) of the Schrödinger equation?

- $\psi(x) = Ae^{-ikx} + Be^{ikx}$
- $\psi(x) = Ae^{-kx} + Be^{kx}$
- $\psi(x) = A \sin 3kx + B \cos 5kx$
- $\psi(x) = A \sin 3kx + B \sin 5kx$
- $\psi(x) = A \tan kx$

Introduction: This problem involves identifying which of the provided functions are valid solutions to the time-independent Schrödinger equation (TISE) in one dimension. A function qualifies as an acceptable solution if it satisfies the TISE:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

and is also physically admissible.

Criteria for Acceptability of a Wavefunction: A wavefunction $\psi(x)$ is considered physically acceptable if it meets the following criteria:

1. It must be single-valued for all x .
2. It must be continuous and have continuous first derivatives.
3. It must be normalizable: $\int |\psi(x)|^2 dx < \infty$ over the domain.
4. It must be finite everywhere in the domain (no divergences).
5. It must satisfy the boundary conditions of the physical problem.

We analyze each function based on these criteria and whether it satisfies the TISE for a given energy eigenvalue.

Solution:

1. $\psi(x) = Ae^{-ikx} + Be^{ikx}$

This represents the general solution for a free particle with energy $E = \frac{\hbar^2 k^2}{2m}$. Although it is not normalizable over infinite space, it is commonly used in scattering theory and considered acceptable as a formal solution.

Acceptable solution.

2. $\psi(x) = Ae^{-kx} + Be^{kx}$

Contains an exponentially growing term Be^{kx} , which diverges as $x \rightarrow \infty$, violating the normalizability criterion. Acceptable only if $B = 0$ and x is constrained, such as in bound state decaying wavefunctions.

Not acceptable in general form.

3. $\psi(x) = A \sin 3kx + B \cos 5kx$

This function is a linear combination of sine and cosine terms with different wave numbers (and hence different energies). Such a superposition does not satisfy a single-energy TISE.

Not acceptable as a single eigenfunction.

4. $\psi(x) = A \sin 3kx + B \sin 5kx$

Similarly, this is a superposition of solutions with different wave numbers, and thus different energies. It does not satisfy the TISE for a specific energy eigenvalue.

Not acceptable as a single eigenfunction.

5. $\psi(x) = A \tan kx$

The tangent function has singularities at $x = \frac{(2n+1)\pi}{2k}$, where it diverges. This violates the finiteness and continuity requirements of acceptable wavefunctions.

Not acceptable solution.

Conclusion: The only acceptable solution among the provided options, from the standpoint of the time-independent Schrödinger equation for a single energy eigenvalue, is:

- $\psi(x) = Ae^{-ikx} + Be^{ikx}$

All others are disqualified due to non-normalizability, divergence, or being superpositions of different energy eigenfunctions.

A/P

41 A beam of particles of energy 9 eV is incident on a potential step 8 eV high from the left. What percentage of particles will reflect back?

Introduction:

In quantum mechanics, the reflection and transmission of particles at a potential step is a fundamental problem. When a particle encounters a potential step, part of the wave function is reflected, and part is transmitted. The reflection coefficient (R) gives the probability of the particle being reflected.

Solution:

The energy of the incident particles is $E = 9 \text{ eV}$, and the height of the potential step is $V_0 = 8 \text{ eV}$. The reflection coefficient (R) is given by:

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

where k_1 and k_2 are the wave numbers of the particle in the regions before and after the potential step, respectively.

The wave number k is related to the energy E and the potential V by:

$$k = \sqrt{\frac{2m(E - V)}{\hbar^2}}$$

For the region before the potential step ($E = 9 \text{ eV}$ and $V = 0 \text{ eV}$):

$$k_1 = \sqrt{\frac{2m(9 \text{ eV})}{\hbar^2}}$$

For the region after the potential step ($E = 9 \text{ eV}$ and $V = 8 \text{ eV}$):

$$k_2 = \sqrt{\frac{2m(9 \text{ eV} - 8 \text{ eV})}{\hbar^2}} = \sqrt{\frac{2m(1 \text{ eV})}{\hbar^2}}$$

The ratio of the wave numbers is:

$$\frac{k_1}{k_2} = \frac{\sqrt{9 \text{ eV}}}{\sqrt{1 \text{ eV}}} = 3$$

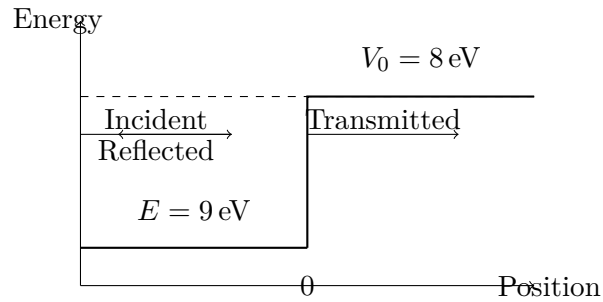
Substituting into the reflection coefficient formula:

$$R = \left(\frac{3 - 1}{3 + 1} \right)^2 = \left(\frac{2}{4} \right)^2 = \left(\frac{1}{2} \right)^2 = 0.25$$

Therefore, the reflection percentage is:

$$R \times 100\% = 0.25 \times 100\% = 25\%$$

The following diagram illustrates the potential step and the wave function behavior:



Conclusion:

The reflection coefficient indicates that 25% of the particles will reflect back when a beam of particles with energy 9 eV encounters a potential step of 8 eV. This result highlights the wave nature of particles, where partial reflection and transmission occur due to quantum mechanical effects.

Applications:

1. **Tunneling in Semiconductors:** Quantum tunneling is crucial in the operation of semiconductor devices such as diodes and transistors.
2. **Scanning Tunneling Microscopy (STM):** STM relies on the quantum tunneling of electrons to image surfaces at the atomic level.
3. **Nuclear Fusion:** Quantum tunneling allows particles to overcome the Coulomb barrier, facilitating nuclear reactions in stars and experimental fusion reactors.

42 Estimate the size of hydrogen atom and the ground state energy from the uncertainty principle.

Introduction: The problem requires an estimation of the characteristic size (Bohr radius) and ground state energy of a hydrogen atom using the Heisenberg uncertainty principle. The hydrogen atom consists of an electron bound to a proton via Coulomb attraction. We aim to estimate:

- The approximate radius r of the hydrogen atom,
- The ground state energy E of the electron.

We assume a non-relativistic quantum mechanical model and apply the uncertainty relation $\Delta x \Delta p \sim \hbar$.

Solution:

Let the electron be confined within a region of size r , so the uncertainty in position is $\Delta x \sim r$. Then the uncertainty in momentum is:

$$\Delta p \sim \frac{\hbar}{r} \text{ order of magnitude is satisfied even when we don't take } 1/2 \text{ as a factor}$$

The kinetic energy of the electron can be approximated using:

$$T \sim \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2mr^2},$$

where m is the mass of the electron.

The potential energy due to Coulomb attraction between the proton and the electron is:

$$V \sim -\frac{e^2}{4\pi\epsilon_0 r},$$

where e is the elementary charge and ϵ_0 is the vacuum permittivity.

The total energy of the electron is approximately:

$$E(r) = T + V \sim \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r}.$$

To find the equilibrium (ground state), we minimize $E(r)$ with respect to r :

$$\frac{dE}{dr} = -\frac{\hbar^2}{mr^3} + \frac{e^2}{4\pi\epsilon_0 r^2} = 0.$$

The second derivative greater than 0, confirms a minimum.

Solving for r :

$$\frac{\hbar^2}{mr^3} = \frac{e^2}{4\pi\epsilon_0 r^2} \Rightarrow r = \frac{4\pi\epsilon_0 \hbar^2}{me^2}.$$

This is the Bohr radius:

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \approx 5.29 \times 10^{-11} \text{ m}.$$

Substitute $r = a_0$ into the expression for energy:

$$E = \frac{\hbar^2}{2ma_0^2} - \frac{e^2}{4\pi\epsilon_0 a_0}.$$

This gives the ground state energy:

$$E_0 = -13.6 \text{ eV}.$$

Conclusion: By applying the uncertainty principle, we estimate the size of the hydrogen atom to be approximately $a_0 = 5.29 \times 10^{-11} \text{ m}$, known as the Bohr radius. The ground state energy is approximately $E_0 = -13.6 \text{ eV}$, consistent with experimental results and Bohr's model.

A/P

43 Write down the Hamiltonian operator for a linear harmonic oscillator. Show that the energy eigenvalue of the same can be given by $E_n = (n + \frac{1}{2}) \hbar\omega_0$ at energy state n with ω_0 being the natural frequency of vibration of the linear oscillator. Prove that $n = 0$ energy state has a wave function of typical Gaussian form.

Introduction: The problem involves analyzing the quantum harmonic oscillator. We are asked to:

- Write the Hamiltonian operator for a linear harmonic oscillator.
- Derive the energy eigenvalues, demonstrating the quantized form $E_n = (n + \frac{1}{2}) \hbar\omega_0$.
- Show that the ground state wavefunction ($n = 0$) has a Gaussian form.

Assumptions include a one-dimensional oscillator and standard canonical quantization with position operator $\hat{x}$ and momentum operator $\hat{p}$ satisfying $[\hat{x}, \hat{p}] = i\hbar$.

Solution:

The Hamiltonian for a one-dimensional quantum harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2.$$

This represents the total energy of the system the sum of kinetic and potential energies in quantum mechanical form.

To simplify the problem and reveal its underlying algebraic structure, we introduce ladder (creation and annihilation) operators:

$$\begin{aligned}\hat{a} &= \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega_0} \hat{p} \right), \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega_0} \hat{p} \right).\end{aligned}$$

These satisfy the commutation relation:

$$[\hat{a}, \hat{a}^\dagger] = 1.$$

Ladder operators provide an elegant way to analyze the harmonic oscillator because they allow us to raise or lower the energy levels of the system in discrete steps, corresponding to the quantized nature of energy in quantum mechanics.

In terms of these operators, the Hamiltonian becomes:

$$\hat{H} = \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right).$$

The number operator is defined as $\hat{n} = \hat{a}^\dagger \hat{a}$, and its eigenstates $|n\rangle$ satisfy:

$$\hat{n} |n\rangle = n |n\rangle, \quad n = 0, 1, 2, \dots$$

Hence, the energy eigenvalues are:

$$E_n = \hbar\omega_0 \left(n + \frac{1}{2} \right).$$

This result shows that the energy levels are quantized and equally spaced, with a minimum energy of $\frac{1}{2}\hbar\omega_0$, known as the zero-point energy. This non-zero minimum energy reflects the Heisenberg uncertainty principle: even in the ground state, the particle cannot have both definite position and momentum.

Now consider the ground state $|0\rangle$, which satisfies:

$$\hat{a} |0\rangle = 0.$$

Using the coordinate representation, we have:

$$\begin{aligned}\hat{x} &= x, \\ \hat{p} &= -i\hbar \frac{d}{dx}.\end{aligned}$$

Thus the annihilation operator becomes:

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}} \left(x + \frac{\hbar}{m\omega_0} \frac{d}{dx} \right).$$

Apply $\hat{a}$ to the ground state wavefunction $\psi_0(x)$:

$$\hat{a}\psi_0(x) = 0 \quad \Rightarrow \quad \left(x + \frac{\hbar}{m\omega_0} \frac{d}{dx} \right) \psi_0(x) = 0.$$

Solving this differential equation:

$$\frac{d\psi_0}{dx} = -\frac{m\omega_0}{\hbar} x \psi_0(x).$$

This is a separable differential equation. Integrating both sides:

$$\begin{aligned}\int \frac{1}{\psi_0} d\psi_0 &= -\frac{m\omega_0}{\hbar} \int x dx, \\ \ln \psi_0 &= -\frac{m\omega_0}{2\hbar} x^2 + C, \\ \psi_0(x) &= A e^{-\frac{m\omega_0}{2\hbar} x^2},\end{aligned}$$

where $A = e^C$ is the normalization constant.

To normalize, we impose:

$$\int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = 1 \Rightarrow A = \left(\frac{m\omega_0}{\pi\hbar} \right)^{1/4}.$$

Conclusion: The Hamiltonian operator for a linear harmonic oscillator is $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2$. Its energy eigenvalues are quantized as $E_n = (n + \frac{1}{2})\hbar\omega_0$, reflecting the discrete and equally spaced energy levels characteristic of quantum oscillators. The ground state ($n = 0$) wavefunction is of Gaussian form:

$$\psi_0(x) = \left(\frac{m\omega_0}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega_0}{2\hbar} x^2}.$$

This confirms both the quantized energy spectrum and the Gaussian nature of the ground state in quantum harmonic oscillators. Moreover, excited states can be generated by applying the creation operator repeatedly on the ground state.

44 Prove that Bohr hydrogen atom approaches classical conditions, when n becomes very large and small quantum jumps are involved.

Introduction:

The correspondence principle, formulated by Niels Bohr, states that the behavior of systems described by quantum mechanics replicates classical physics in the limit of large quantum numbers. For the Bohr model of the hydrogen atom, this principle can be demonstrated by showing that the energy levels become closely spaced and the frequency of radiation approaches the classical orbital frequency as n becomes very large.

Solution:

1. Energy Levels in Bohr Model:

The energy levels of a hydrogen atom in the Bohr model are given by:

$$E_n = -\frac{13.6 \text{ eV}}{n^2}$$

where n is the principal quantum number.

2. Frequency of Radiation:

When an electron transitions from a higher energy level n_i to a lower energy level n_f , the frequency of the emitted photon is:

$$f = \frac{E_i - E_f}{h}$$

Substituting the energy levels:

$$f = \frac{-\frac{13.6 \text{ eV}}{n_i^2} + \frac{13.6 \text{ eV}}{n_f^2}}{h}$$

Let $n_i = n$ and $n_f = n - \Delta n$ where Δn is small compared to n . Then,

$$f = \frac{13.6 \text{ eV}}{h} \left(\frac{1}{(n - \Delta n)^2} - \frac{1}{n^2} \right)$$

For large n and small Δn , we can use the binomial approximation:

$$(n - \Delta n)^2 \approx n^2 - 2n\Delta n$$

So,

$$\frac{1}{(n - \Delta n)^2} \approx \frac{1}{n^2} \left(1 + \frac{2\Delta n}{n} \right)$$

Therefore,

$$f \approx \frac{13.6 \text{ eV}}{h} \left(\frac{1}{n^2} - \frac{1}{n^2} \left(1 + \frac{2\Delta n}{n} \right) \right) = \frac{13.6 \text{ eV}}{h} \frac{2\Delta n}{n^3}$$

3. Classical Orbital Frequency:

The classical orbital frequency $f_{\text{classical}}$ of an electron in the n th orbit is given by:

$$f_{\text{classical}} = \frac{\omega}{2\pi} = \frac{v}{2\pi r}$$

Using Bohr's model, $v = \frac{e^2}{2\epsilon_0 h} \frac{1}{n}$ and $r = \frac{4\pi\epsilon_0 h^2 n^2}{e^2 m}$, we get:

$$f_{\text{classical}} = \frac{\left(\frac{e^2}{2\epsilon_0 h} \frac{1}{n}\right)}{2\pi \left(\frac{4\pi\epsilon_0 h^2 n^2}{e^2 m}\right)} = \frac{e^4 m}{16\pi^3 \epsilon_0^2 h^3} \frac{1}{n^3}$$

4. Comparison and Conclusion:

For large n ,

$$f \approx \frac{13.6 \text{ eV}}{h} \frac{2\Delta n}{n^3} = f_{\text{classical}} \Delta n$$

Thus, the frequency of the radiation approaches the classical orbital frequency when the quantum number n is very large, confirming Bohr's correspondence principle.

Conclusion:

As the quantum number n becomes very large, the energy levels of the Bohr hydrogen atom become closely spaced, and the frequency of emitted radiation for small quantum jumps approaches the classical orbital frequency. This demonstrates that the Bohr model converges to classical physics in the limit of large quantum numbers, highlighting the correspondence principle. Practical applications include understanding atomic spectra and transitions in high-energy physics and astrophysics.

45 Find the probability current density for the wave function $\Psi(x, t) = [Ae^{ipx/\hbar} + Be^{-ipx/\hbar}] e^{-ip^2t/2m\hbar}$. Interpret the result physically.

Introduction:

In quantum mechanics, the probability current density $\mathbf{j}(x, t)$ represents the flow of probability associated with the wave function $\Psi(x, t)$. It is defined as:

$$\mathbf{j}(x, t) = \frac{\hbar}{2mi} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right)$$

where Ψ^* is the complex conjugate of Ψ .

Solution:

Given the wave function:

$$\Psi(x, t) = [Ae^{ipx/\hbar} + Be^{-ipx/\hbar}] e^{-ip^2t/2m\hbar}$$

First, find the partial derivatives of Ψ and Ψ^* with respect to x .

1. Partial Derivative of Ψ with Respect to x :

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x} [(Ae^{ipx/\hbar} + Be^{-ipx/\hbar}) e^{-ip^2t/2m\hbar}]$$

Since $e^{-ip^2t/2m\hbar}$ is a constant with respect to x :

$$\begin{aligned} \frac{\partial \Psi}{\partial x} &= e^{-ip^2t/2m\hbar} \left[\frac{\partial}{\partial x} (Ae^{ipx/\hbar} + Be^{-ipx/\hbar}) \right] \\ &= e^{-ip^2t/2m\hbar} \left[\frac{ip}{\hbar} Ae^{ipx/\hbar} - \frac{ip}{\hbar} Be^{-ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} e^{-ip^2t/2m\hbar} [Ae^{ipx/\hbar} - Be^{-ipx/\hbar}] \end{aligned}$$

2. Partial Derivative of Ψ^* with Respect to x :

The complex conjugate of $\Psi(x, t)$ is:

$$\Psi^*(x, t) = [A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}] e^{ip^2t/2m\hbar}$$

$$\begin{aligned} \frac{\partial \Psi^*}{\partial x} &= e^{ip^2t/2m\hbar} \left[\frac{\partial}{\partial x} (A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}) \right] \\ &= e^{ip^2t/2m\hbar} \left[-\frac{ip}{\hbar} A^*e^{-ipx/\hbar} + \frac{ip}{\hbar} B^*e^{ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} e^{ip^2t/2m\hbar} [-A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}] \end{aligned}$$

3. Probability Current Density:

Using the definition of $\mathbf{j}(x, t)$:

$$\mathbf{j}(x, t) = \frac{\hbar}{2mi} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right)$$

Substitute Ψ , Ψ^* , and their derivatives:

$$\begin{aligned} \Psi^* \frac{\partial \Psi}{\partial x} &= \left[A^* e^{-ipx/\hbar} + B^* e^{ipx/\hbar} \right] e^{ip^2 t/2m\hbar} \cdot \frac{ip}{\hbar} e^{-ip^2 t/2m\hbar} \left[A e^{ipx/\hbar} - B e^{-ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} \left[A^* e^{-ipx/\hbar} A e^{ipx/\hbar} - A^* e^{-ipx/\hbar} B e^{-ipx/\hbar} + B^* e^{ipx/\hbar} A e^{ipx/\hbar} - B^* e^{ipx/\hbar} B e^{-ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} \left[A^* A - A^* B e^{-2ipx/\hbar} + B^* A e^{2ipx/\hbar} - B^* B \right] \end{aligned}$$

Similarly,

$$\begin{aligned} \Psi \frac{\partial \Psi^*}{\partial x} &= \left[A e^{ipx/\hbar} + B e^{-ipx/\hbar} \right] e^{-ip^2 t/2m\hbar} \cdot \frac{ip}{\hbar} e^{ip^2 t/2m\hbar} \left[-A^* e^{-ipx/\hbar} + B^* e^{ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} \left[A e^{ipx/\hbar} (-A^* e^{-ipx/\hbar}) + A e^{ipx/\hbar} B^* e^{ipx/\hbar} + B e^{-ipx/\hbar} (-A^* e^{-ipx/\hbar}) + B e^{-ipx/\hbar} B^* e^{ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} \left[-AA^* + AB^* e^{2ipx/\hbar} - BA^* e^{-2ipx/\hbar} + BB^* \right] \end{aligned}$$

Therefore, the probability current density is:

$$\begin{aligned} \mathbf{j}(x, t) &= \frac{\hbar}{2mi} \left[\frac{ip}{\hbar} \left(A^* A - A^* B e^{-2ipx/\hbar} + B^* A e^{2ipx/\hbar} - B^* B \right) - \frac{ip}{\hbar} \left(-AA^* + AB^* e^{2ipx/\hbar} - BA^* e^{-2ipx/\hbar} + BB^* \right) \right] \\ &= \frac{\hbar}{2mi} \cdot \frac{2ip}{\hbar} (A^* A - B^* B) \\ \mathbf{j}(x, t) &= \frac{p}{m} (A^* A - B^* B) \end{aligned}$$

Conclusion:

The probability current density for the given wave function is:

$$\mathbf{j}(x, t) = \frac{p}{m} (A^* A - B^* B)$$

Interpretation:

This result indicates that the probability current density depends on the coefficients A and B . If $|A|^2 = |B|^2$, the probability current density $\mathbf{j}(x, t)$ is zero, implying no net flow of probability. If $|A|^2 \neq |B|^2$, there is a net flow of probability in the direction of the momentum p .

This reflects the physical interpretation that the probability current density represents the flow of probability for a particle described by the wave function $\Psi(x, t)$. The terms $|A|^2$ and $|B|^2$ represent the probabilities of the particle moving in positive and negative directions, respectively. The difference between these probabilities determines the net flow of probability in the system.

A/P

46 A particle is described by the wave function $\Psi(x) = \left(\frac{\pi}{2}\right)^{-1/4} e^{-ax^2/2}$. Calculate Δx and Δp for the particle, and verify the uncertainty relation $\Delta x \Delta p = \frac{\hbar}{2}$.

Introduction: The given wave function is a Gaussian:

$$\Psi(x) = \left(\frac{\pi}{2}\right)^{-1/4} e^{-ax^2/2},$$

where $a > 0$ is a real constant. We are asked to find the uncertainties Δx and Δp and verify the Heisenberg uncertainty relation:

$$\Delta x \Delta p \geq \frac{\hbar}{2}.$$

To compute uncertainties, we need:

1. $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$,
2. $\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$,

where $\langle x \rangle$ and $\langle p \rangle$ are expectation values of position and momentum, respectively.

Solution:

1. Expectation values:

Since $\Psi(x)$ is an even function and complete integrand is odd function:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x)|^2 dx = 0.$$

For momentum, we use $\hat{p} = -i\hbar \frac{d}{dx}$:

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \left(-i\hbar \frac{d}{dx} \right) \Psi(x) dx.$$

Since $\frac{d\Psi}{dx} = -ax\Psi(x)$:

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x) (-i\hbar) (-ax) \Psi(x) dx = i\hbar a \int_{-\infty}^{\infty} x |\Psi(x)|^2 dx = 0,$$

because the integrand is odd.

2. Compute $\langle x^2 \rangle$:

$$|\Psi(x)|^2 = \left(\frac{\pi}{2}\right)^{-1/2} e^{-ax^2}.$$

Then,

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\Psi(x)|^2 dx = \left(\frac{\pi}{2}\right)^{-1/2} \int_{-\infty}^{\infty} x^2 e^{-ax^2} dx.$$

Using the standard integral:

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}},$$

we get:

$$\langle x^2 \rangle = \left(\frac{\pi}{2}\right)^{-1/2} \cdot \frac{\sqrt{\pi}}{2a^{3/2}} = \frac{1}{2a}.$$

Thus,

$$\Delta x = \sqrt{\langle x^2 \rangle} = \sqrt{\frac{1}{2a}} = \frac{1}{\sqrt{2a}}.$$

3. Compute $\langle p^2 \rangle$:

We calculate $\langle p^2 \rangle = \langle -\hbar^2 \frac{d^2}{dx^2} \rangle$:

First, compute derivatives:

$$\frac{d\Psi}{dx} = -ax\Psi(x), \quad \frac{d^2\Psi}{dx^2} = -a\Psi(x) - ax(-ax)\Psi(x) = (-a + a^2x^2)\Psi(x).$$

So:

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \left(-\hbar^2 \frac{d^2}{dx^2} \right) \Psi(x) dx = -\hbar^2 \int_{-\infty}^{\infty} |\Psi(x)|^2 (-a + a^2x^2) dx.$$

$$\langle p^2 \rangle = \hbar^2 \int_{-\infty}^{\infty} |\Psi(x)|^2 (a - a^2x^2) dx = \hbar^2 \left(a \int_{-\infty}^{\infty} |\Psi(x)|^2 dx - a^2 \int_{-\infty}^{\infty} x^2 |\Psi(x)|^2 dx \right).$$

Using $\int |\Psi(x)|^2 dx = 1$ and $\langle x^2 \rangle = \frac{1}{2a}$:

$$\langle p^2 \rangle = \hbar^2 \left(a - a^2 \cdot \frac{1}{2a} \right) = \hbar^2 \left(a - \frac{a}{2} \right) = \frac{a\hbar^2}{2}.$$

Therefore:

$$\Delta p = \sqrt{\frac{a\hbar^2}{2}} = \frac{\hbar\sqrt{a}}{\sqrt{2}}.$$

4. Uncertainty product:

$$\Delta x \Delta p = \frac{1}{\sqrt{2a}} \cdot \frac{\hbar\sqrt{a}}{\sqrt{2}} = \frac{\hbar\sqrt{a}}{\sqrt{2a} \cdot \sqrt{2}} = \frac{\hbar\sqrt{a}}{2\sqrt{a}} = \frac{\hbar}{2}.$$

Conclusion: The uncertainties in position and momentum are:

$$\Delta x = \frac{1}{\sqrt{2a}}, \quad \Delta p = \frac{\hbar\sqrt{a}}{\sqrt{2}},$$

and their product satisfies the Heisenberg uncertainty principle exactly:

$$\Delta x \Delta p = \frac{\hbar}{2}.$$

This confirms the wave function is a minimum uncertainty Gaussian state.

47 A beam of 12eV electron is incident on a potential barrier of height 25eV and width 0.05 nm. Calculate the transmission coefficient.

Solution:

Given:

- Electron energy, $E = 12 \text{ eV}$
- Barrier height, $V_0 = 25 \text{ eV}$
- Barrier width, $a = 0.05 \text{ nm} = 5 \times 10^{-11} \text{ m}$

For a rectangular barrier with $E < V_0$, the transmission coefficient is:

$$T = \left[1 + \frac{V_0^2 \sinh^2(\kappa a)}{4E(V_0 - E)} \right]^{-1}$$

where

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

Constants:

$$m = 9.11 \times 10^{-31} \text{ kg}, \quad \hbar = 1.055 \times 10^{-34} \text{ Js}, \quad 1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$$

Compute:

$$\kappa = \frac{\sqrt{2 \cdot 9.11 \times 10^{-31} \cdot 13 \cdot 1.602 \times 10^{-19}}}{1.055 \times 10^{-34}} = \frac{\sqrt{3.785 \times 10^{-48}}}{1.055 \times 10^{-34}} \approx \frac{6.15 \times 10^{-24}}{1.055 \times 10^{-34}} \approx 5.83 \times 10^{10} \text{ m}^{-1}$$

Now:

$$\kappa a = 5.83 \times 10^{10} \cdot 5 \times 10^{-11} = 2.915$$

$$\sinh(\kappa a) \approx \sinh(2.915) \approx 9.18$$

Now plug into the full expression:

$$T = \left[1 + \frac{(25)^2 \cdot (9.18)^2}{4 \cdot 12 \cdot 13} \right]^{-1} = \left[1 + \frac{625 \cdot 84.29}{624} \right]^{-1} = \left[1 + \frac{52681.25}{624} \right]^{-1} \approx [1 + 84.42]^{-1}$$

$$T \approx \frac{1}{85.42} \approx 0.0117$$

Answer: The transmission coefficient is approximately 0.012, meaning there is about a 1.2% probability of the electron tunneling through the barrier.

- 48 Solve the Schrödinger equation for a step potential and calculate the transmission and reflection coefficients for the case when the kinetic energy of the particle E_0 is greater than the potential energy V (i.e., $E_0 > V$).

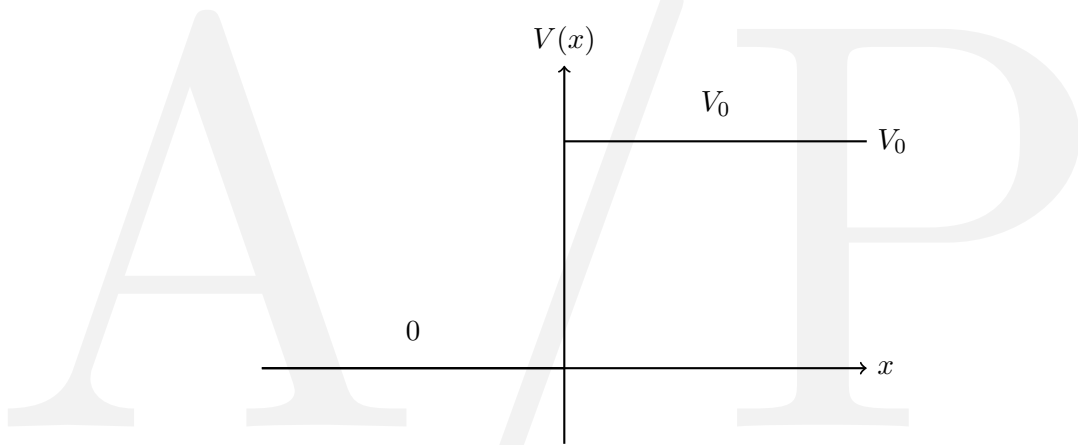
Introduction:

The step potential is a fundamental problem in quantum mechanics that illustrates the behavior of a particle encountering a sudden change in potential energy. This problem is essential for understanding phenomena such as quantum tunneling and reflection.

Consider a particle encountering a step potential:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x \geq 0 \end{cases}$$

Below is a diagram illustrating the step potential:



Solution:

Consider a particle encountering a step potential:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x \geq 0 \end{cases}$$

The Schrödinger equation in regions where $V(x)$ is constant is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

For $x < 0$ (Region I), where $V(x) = 0$:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E_0\psi(x)$$

The general solution is:

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

where:

$$k_1 = \sqrt{\frac{2mE_0}{\hbar^2}}$$

For $x \geq 0$ (Region II), where $V(x) = V_0$:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E_0\psi(x)$$

This simplifies to:

$$\frac{d^2\psi(x)}{dx^2} = k_2^2\psi(x)$$

where:

$$k_2 = \sqrt{\frac{2m(E_0 - V_0)}{\hbar^2}}$$

The general solution is:

$$\psi_{II}(x) = Ce^{ik_2x}$$

Since we consider the particle coming from the left and moving to the right, there will be no wave traveling to the left in Region II ($D = 0$):

$$\psi_{II}(x) = Ce^{ik_2x}$$

Boundary Conditions:

At $x = 0$, the wavefunctions and their first derivatives must be continuous:

$$\begin{aligned}\psi_I(0) &= \psi_{II}(0) \\ \left. \frac{d\psi_I}{dx} \right|_{x=0} &= \left. \frac{d\psi_{II}}{dx} \right|_{x=0}\end{aligned}$$

Applying these conditions:

1. Continuity of wavefunction:

$$A + B = C$$

2. Continuity of derivative:

$$ik_1A - ik_1B = ik_2C$$

Solving these equations for A , B , and C :

From the first equation:

$$C = A + B$$

Substituting into the second equation:

$$ik_1A - ik_1B = ik_2(A + B)$$

Rearranging:

$$k_1A - k_1B = k_2A + k_2B$$

$$(k_1 - k_2)A = (k_1 + k_2)B$$

$$\frac{A}{B} = \frac{k_1 + k_2}{k_1 - k_2}$$

Therefore, the reflection coefficient R is:

$$R = \left| \frac{B}{A} \right|^2 = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2$$

To correctly compute the transmission coefficient T , we must account for the difference in group velocities across regions. This gives:

$$T = \frac{k_2}{k_1} \left| \frac{C}{A} \right|^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

Conclusion:

For a particle encountering a step potential with $E_0 > V_0$, the reflection and transmission coefficients are:

$$R = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2, \quad T = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

These coefficients describe the probability of the particle being reflected or transmitted at the potential step and obey the conservation law $R + T = 1$.

A/P

49 Write the wave functions for a particle on both sides of a step potential, for $E > V_0$:

$$V(x) = \begin{cases} V_0, & x > 0 \\ 0, & x < 0 \end{cases}$$

Interpret the results physically.

Introduction: This problem involves a quantum particle encountering a 1D step potential. The potential energy function is piecewise constant, and the total energy of the particle satisfies $E > V_0$. Our goal is to determine the wavefunctions in both regions and interpret the behavior of the particle, including any reflection or transmission effects due to the step.

Solution:

The time-independent Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).$$

We solve this separately in regions I ($x < 0$) and II ($x > 0$).

Region I: $x < 0$ (where $V(x) = 0$)

The Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi,$$

which simplifies to:

$$\frac{d^2\psi}{dx^2} + k_1^2\psi = 0, \quad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar}.$$

General solution:

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}.$$

Here, Ae^{ik_1x} represents the incident wave, and Be^{-ik_1x} is the reflected wave.

Region II: $x > 0$ (where $V(x) = V_0$)

The Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0\psi = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k_2^2\psi = 0,$$

where

$$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}.$$

General solution:

$$\psi_{II}(x) = Ce^{ik_2x}.$$

We exclude the term De^{-ik_2x} because it would represent a wave incoming from $x \rightarrow \infty$, which contradicts the physical setup of a wave incident from the left.

Boundary Conditions:

Continuity of the wavefunction and its derivative at $x = 0$:

$$\begin{aligned}\psi_I(0) &= \psi_{II}(0) \Rightarrow A + B = C, \\ \psi'_I(0) &= \psi'_{II}(0) \Rightarrow ik_1(A - B) = ik_2C.\end{aligned}$$

Solving this system:

$$\begin{aligned}A + B &= C \\ k_1(A - B) &= k_2(A + B)\end{aligned}$$

Solving for B/A and C/A :

$$\begin{aligned}\frac{B}{A} &= \frac{k_1 - k_2}{k_1 + k_2}, \\ \frac{C}{A} &= \frac{2k_1}{k_1 + k_2}.\end{aligned}$$

Interpretation:

Even though the energy $E > V_0$, the particle has a finite probability of being reflected. The reflection coefficient R and transmission coefficient T are given by:

$$\begin{aligned}R &= \left| \frac{B}{A} \right|^2 = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2, \\ T &= \frac{k_2}{k_1} \left| \frac{C}{A} \right|^2 = \frac{4k_1k_2}{(k_1 + k_2)^2}.\end{aligned}$$

Note that $R + T = 1$, as required by probability conservation.

Physically, even when the particle has enough energy to surpass the potential step, there is a non-zero probability of reflection due to the abrupt change in potential, a purely quantum mechanical phenomenon with no classical analog.

Conclusion: The wavefunctions in each region are:

$$\begin{aligned}\psi_I(x) &= Ae^{ik_1x} + Be^{-ik_1x}, \quad x < 0, \\ \psi_{II}(x) &= Ce^{ik_2x}, \quad x > 0.\end{aligned}$$

Despite having energy $E > V_0$, the particle experiences partial reflection and transmission due to the discontinuity in potential. This highlights the wave nature of particles in quantum mechanics and the non-classical behavior at potential boundaries.

50 Normalize the 1s state of the hydrogen atom in the ground state and calculate the expectation value of position

Introduction:

The hydrogen atom's ground state (1s) wave function in spherical coordinates is given by:

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

where $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ is the Bohr radius. This function includes both the radial and angular dependence. For the 1s state, the angular dependence is constant: $Y_{00} = \frac{1}{\sqrt{4\pi}}$, and hence we focus primarily on the radial part for normalization and expectation value computations.

Our goal is to: 1. Normalize the wave function, and 2. Compute the expectation value of the radial distance $\langle r \rangle$.

1. Normalization of the wave function:

The normalization condition in three dimensions is:

$$\int |\psi_{100}(r, \theta, \phi)|^2 d^3r = 1$$

In spherical coordinates, this becomes:

$$\int_0^{2\pi} \int_0^\pi \int_0^\infty |\psi_{100}(r)|^2 r^2 \sin \theta dr d\theta d\phi = 1$$

Substituting $\psi_{100}(r) = Ae^{-r/a_0}$, we write:

$$\int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \int_0^\infty |A|^2 e^{-2r/a_0} r^2 dr = 1$$

Evaluating the angular integrals:

$$\int_0^{2\pi} d\phi = 2\pi, \quad \int_0^\pi \sin \theta d\theta = 2$$

So the normalization condition becomes:

$$4\pi |A|^2 \int_0^\infty e^{-2r/a_0} r^2 dr = 1$$

Using the standard integral:

$$\int_0^\infty r^2 e^{-2r/a_0} dr = \left(\frac{a_0}{2}\right)^3 \cdot \int_0^\infty x^2 e^{-x} dx = \frac{a_0^3}{8} \cdot 2 = \frac{a_0^3}{4}$$

Hence:

$$4\pi |A|^2 \cdot \frac{a_0^3}{4} = 1 \quad \Rightarrow \quad |A|^2 \pi a_0^3 = 1 \quad \Rightarrow \quad |A| = \frac{1}{\sqrt{\pi a_0^3}}$$

So the normalized wave function is:

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

2. Expectation value of position $\langle r \rangle$:

The expectation value of the position is given by:

$$\langle r \rangle = \int_0^{2\pi} \int_0^\pi \int_0^\infty \psi_{100}^*(r) r \psi_{100}(r) r^2 \sin \theta dr d\theta d\phi$$

Substitute the normalized wave function:

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

Evaluate the angular integrals:

$$\int_0^{2\pi} d\phi = 2\pi, \quad \int_0^\pi \sin \theta d\theta = 2$$

So:

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

Using the standard integral:

$$\int_0^\infty r^3 e^{-2r/a_0} dr = \frac{6}{(2/a_0)^4} = \frac{3a_0^4}{4}$$

Then:

$$\langle r \rangle = \frac{2}{a_0^3} \cdot \frac{3a_0^4}{4} = \frac{3a_0}{2}$$

Conclusion:

- The normalized wave function for the hydrogen atom in the 1s state is:

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

- The expectation value of the radial distance in this state is:

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

This result shows that the average distance of the electron from the nucleus in the ground state is 1.5 times the Bohr radius. This reflects the quantum mechanical nature of the atom, where the electron does not orbit at a fixed radius but has a spread-out probability distribution.

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:

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

Lets 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 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:

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$$

$$\sigma_x \sigma_y = i\sigma_z, \quad \sigma_y \sigma_x = -i\sigma_z$$

$$\sigma_y \sigma_z = i\sigma_x, \quad \sigma_z \sigma_y = -i\sigma_x$$

$$\sigma_z \sigma_x = i\sigma_y, \quad \sigma_x \sigma_z = -i\sigma_y$$

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.

A/P

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:

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

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

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 $\langle r \rangle = \frac{3a_0}{2}$ and $\langle \frac{1}{r} \rangle = \frac{1}{a_0}$. These results are consistent with the quantum mechanical description of the hydrogen atom.

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.

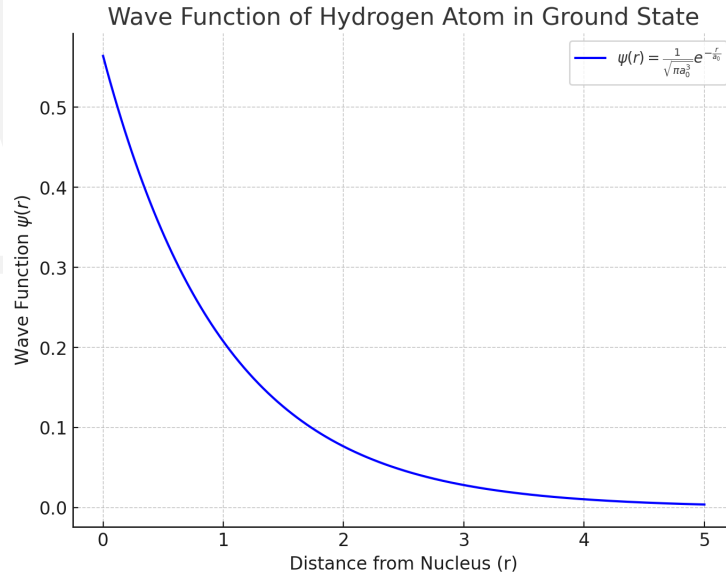
56 Calculate the probability of finding the electron within a distance r_0 of the proton in the ground state.

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:

$$[L_z, L_x] = xp_yyp_z - xp_yzp_y - yp_xyp_z + yp_xzp_y$$

Using the commutation relations:

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

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:

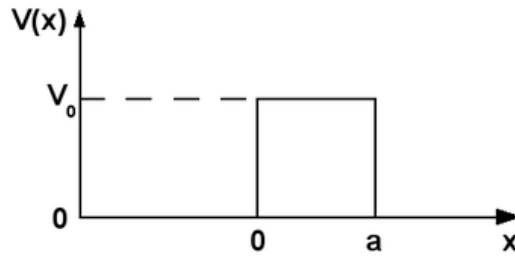


Figure 5: Wave Function for a Particle in a Rectangular Potential Barrier

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**.

A/P

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:

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

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 $p + dp$.

A/P

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:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (7)$$

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:

$$[A, B] = AB - BA. \quad (8)$$

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

$$[\sigma_x, \sigma_y] = \sigma_x \sigma_y - \sigma_y \sigma_x \quad (9)$$

$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (10)$$

Calculating $\sigma_x \sigma_y$:

$$\sigma_x \sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (11)$$

$$= \begin{pmatrix} (0 \cdot 0 + 1 \cdot i) & (0 \cdot -i + 1 \cdot 0) \\ (1 \cdot 0 + 0 \cdot i) & (1 \cdot -i + 0 \cdot 0) \end{pmatrix} \quad (12)$$

$$= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}. \quad (13)$$

Calculating $\sigma_y \sigma_x$:

$$\sigma_y \sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (14)$$

$$= \begin{pmatrix} (0 \cdot 0 + (-i) \cdot 1) & (0 \cdot 1 + (-i) \cdot 0) \\ (i \cdot 0 + 0 \cdot 1) & (i \cdot 1 + 0 \cdot 0) \end{pmatrix} \quad (15)$$

$$= \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}. \quad (16)$$

Now, compute the commutator:

$$[\sigma_x, \sigma_y] = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \quad (17)$$

$$= \begin{pmatrix} i - (-i) & 0 - 0 \\ 0 - 0 & -i - i \end{pmatrix} \quad (18)$$

$$= \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} \quad (19)$$

$$= 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (20)$$

$$= 2i\sigma_z. \quad (21)$$

Thus, we have shown that:

$$[\sigma_x, \sigma_y] = 2i\sigma_z. \quad (22)$$

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:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (23)$$

We are required to prove the following identity:

$$[\sigma^2, \sigma_x] = 0, \quad (24)$$

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

Proof:

First, we compute the square of each Pauli matrix:

$$\sigma_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I, \quad (25)$$

$$\sigma_y^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I, \quad (26)$$

$$\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I. \quad (27)$$

Hence, we find that:

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I, \quad (28)$$

where I is the 2×2 identity matrix.

Now, compute σ^2 :

$$\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = I + I + I = 3I. \quad (29)$$

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

$$[\sigma^2, \sigma_x] = [3I, \sigma_x] \quad (30)$$

$$= 3(I\sigma_x - \sigma_x I). \quad (31)$$

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

$$I\sigma_x = \sigma_x I = \sigma_x. \quad (32)$$

Thus:

$$[\sigma^2, \sigma_x] = 3(\sigma_x - \sigma_x) = 0. \quad (33)$$

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 Schrödingers 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:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x, y, z) = E\psi(x, y, z), \quad (34)$$

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:

$$\psi_{n_x, n_y, n_z}(x, y, z) = \frac{2}{L^{3/2}} \sin\left(\frac{n_x\pi x}{L}\right) \sin\left(\frac{n_y\pi y}{L}\right) \sin\left(\frac{n_z\pi z}{L}\right), \quad (35)$$

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

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

$$E_{n_x, n_y, n_z} = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2). \quad (36)$$

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:

$$n_x^2 + n_y^2 + n_z^2 \leq \frac{2mL^2E}{\hbar^2\pi^2}. \quad (37)$$

The number of such states is:

$$N(E) = 2 \times \frac{1}{8} \cdot \frac{4}{3}\pi n^3 = \frac{1}{3}\pi \left(\frac{2mL^2E}{\hbar^2\pi^2}\right)^{3/2}, \quad (38)$$

where the factor of 2 accounts for spin degeneracy.

Differentiating with respect to E gives the density of states:

$$g(E) = \frac{dN(E)}{dE} = \frac{1}{3}\pi \cdot \frac{3}{2} \left(\frac{2mL^2}{\hbar^2\pi^2} \right)^{3/2} E^{1/2} \quad (39)$$

$$= \frac{\pi}{2} \left(\frac{2mL^2}{\hbar^2\pi^2} \right)^{3/2} E^{1/2}. \quad (40)$$

Now, the density of states per unit volume is:

$$G(E) = \frac{g(E)}{L^3} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2}. \quad (41)$$

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:

$$P(r) = r^2 |R_{21}(r)|^2, \quad (42)$$

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:

$$R_{21}(r) = \frac{1}{4\sqrt{6}a_0^5} r e^{-r/2a_0}, \quad (43)$$

where:

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

Solution:

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

$$P(r) = r^2 |R_{21}(r)|^2 \quad (44)$$

$$= r^2 \left(\frac{1}{4\sqrt{6}a_0^5} r e^{-r/2a_0} \right)^2 \quad (45)$$

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

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:

$$\frac{dP(r)}{dr} = \frac{d}{dr} \left(\frac{r^4}{96a_0^5} e^{-r/a_0} \right) = 0. \quad (47)$$

Applying the product rule:

$$\frac{dP(r)}{dr} = \frac{1}{96a_0^5} \left(4r^3 e^{-r/a_0} - \frac{r^4}{a_0} e^{-r/a_0} \right) = 0. \quad (48)$$

Factor out common terms:

$$\frac{1}{96a_0^5} e^{-r/a_0} r^3 \left(4 - \frac{r}{a_0} \right) = 0. \quad (49)$$

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

$$4 - \frac{r}{a_0} = 0. \quad (50)$$

This gives:

$$r = 4a_0. \quad (51)$$

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:

$$P(4a_0) = \frac{(4a_0)^4}{96a_0^5} e^{-4a_0/a_0}. \quad (52)$$

Simplify:

$$P(4a_0) = \frac{256a_0^4}{96a_0^5} e^{-4} = \frac{256}{96a_0} e^{-4}. \quad (53)$$

Further simplifying:

$$P(4a_0) = \frac{8}{3a_0} e^{-4}. \quad (54)$$

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 $\mathbf{L}$ 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:

$$L^2 = L_x^2 + L_y^2 + L_z^2. \quad (55)$$

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:

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y, \quad (56)$$

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:

$$[L^2, L_x] = 0, \quad [L^2, L_y] = 0, \quad [L^2, L_z] = 0. \quad (57)$$

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 :

$$[H, L^2] = 0, \quad [H, L_z] = 0. \quad (58)$$

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:

$$[\hat{p}_x, \hat{L}_y] = i\hbar\hat{p}_z \quad (59)$$

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:

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}. \quad (60)$$

The angular momentum operator in the y -direction is:

$$\hat{L}_y = \hat{x}\hat{p}_z - \hat{z}\hat{p}_x. \quad (61)$$

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:

$$e^{i(\vec{\sigma} \cdot \hat{n})\theta} = \cos \theta + i(\vec{\sigma} \cdot \hat{n}) \sin \theta. \quad (62)$$

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.

A/P

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:

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

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:

1. A 100 g (0.1 kg) ball confined in a 5 m long box.
2. An oxygen atom ($m \approx 2.66 \times 10^{-26}$ kg) in a 0.2 m box.
3. 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: $m = 0.1$ kg, $L = 5$ 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: $m = 2.66 \times 10^{-26}$ kg, $L = 0.2$ 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: $m = 9.11 \times 10^{-31}$ kg, $L = 10^{-10}$ 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:

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

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:

1. Zero-point energy of 100 g ball in 5 m box: 2.2×10^{-68} J
2. Zero-point energy of oxygen atom in 0.2 m lattice: 5.2×10^{-40} J
3. Zero-point energy of electron in 10^{-10} m atom: 6.02×10^{-18} J or 37.6 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.

A/P