UPSC PHYSICS PYQ SOLUTION
Quantum Mechanics - Part 3

Contents

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.

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 $\frac{\partial\psi}{\partial x}$:

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

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

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

Substitute these into the probability current expression:

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

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

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

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 $\psi(x)$:

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

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

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

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

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.

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 ($A \neq 0$):

$$\sin(kL) = 0$$

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

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 $x \to \infty$, $V(x) \to 0$).

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.

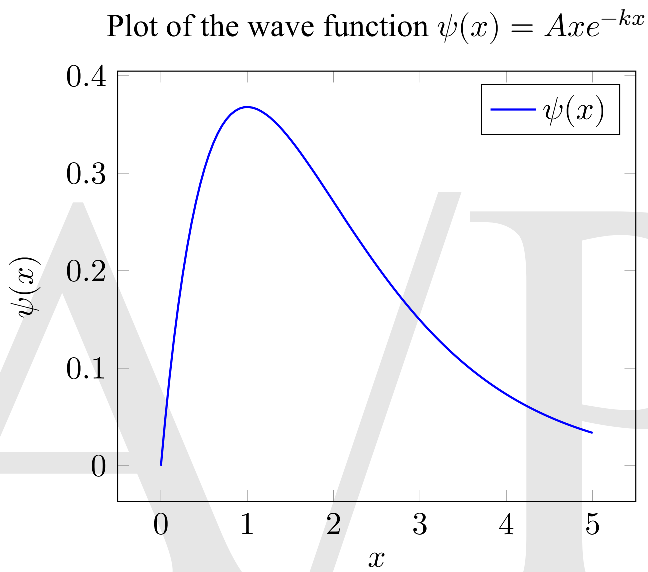

Figure 1: Plot of the wave function $\psi(x) = Axe^{-kx}$

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

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

Now, integrate and set it equal to 1:

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

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 $x \to \infty, V(x) \to 0$).

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:

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

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

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

Since this must hold for all x:

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

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

Now, solve for $V(x)$:

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

Given that as $x \to \infty, V(x) \to 0$: 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 $V(x) = -\frac{\hbar^2 k^2}{m}\left(\frac{1}{x}\right)$.

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:

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

Substituting this into the Schrödinger equation:

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

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

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

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

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

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:

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

Rewriting and simplifying:

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

Introducing the substitution:

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

We obtain:

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

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:

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

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.

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:

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

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:

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

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 $L = 1$ Å $= 1 \times 10^{-10}$ 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 $\hbar = 1.0545718 \times 10^{-34}$ J $\cdot$ s - Electron mass $m = 9.10938356 \times 10^{-31}$ kg - Width $L = 1 \times 10^{-10}$ 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.