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Assignment - 2

Q1) Derive Schrodinger's time independent wave equation.

Ans For a particle of mass m moving in a potential $V(r)$, Schrodinger's time dependent equation is given by

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(r,t) + V(r)\Psi(r,t) \quad -(i)$$

where $\Psi(r,t)$ is the wave function, which depends on position r and time t

$\hbar$ is reduced plank constant

∇^2 is the laplacian operator

$V(r)$ is the potential energy function

The wave function $\Psi(x,t)$ is the product of space function $\psi(x)$ and time function $\varphi(t)$

$$\therefore \Psi(x,t) = \psi(x)\varphi(t) \quad -(ii)$$

Now apply the wave function from equation (ii) to time dependent Schrodinger wave equation (i)

$$i\hbar\psi(x)\frac{d\varphi(t)}{dt} = -\frac{\hbar^2}{2m}\varphi(t)\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\varphi(t) \quad -(iii)$$

In above equation ordinary derivatives are used instead of partial derivatives because each function $\psi(x)$ and $\varphi(t)$ depends on one variable

Now divide equation (iii) by $\psi(x)\varphi(t)$ so.

$$i\hbar \frac{1}{\Psi(t)} \frac{d\Psi(t)}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\Psi(x)} \frac{d^2\Psi(x)}{dx^2} + V(x) \quad \text{--- (iv)}$$

The above equation is known as separation of time -independent part and time independent part of wave equation. The time independent part is known as the energy function operatior i.e

$$E = i\hbar \frac{1}{\Psi(t)} \frac{d\Psi(t)}{dt} \quad \text{--- (V)}$$

$\therefore$ from eq (V) and (iv)

$$E = -\frac{h^2}{2m} \frac{1}{\Psi(x)} \frac{d^2\Psi(x)}{dx^2} + V(x)$$

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

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E-V)\Psi(x) = 0$$

This is time independent Schrodinger wave equation

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Q2.) Derive an equation for energy of a particle enclosed in 1D rigid box or in an infinite potential well.

Ans

We define the potential $(V(x))$ as follows

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

Here, L is the length of box. The particle is only allowed to exist in region $0 \leq x \leq L$ and infinite potential outside the region prevents particle from escaping.

Inside box $V(x) = 0$

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

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

$$K.F = \frac{\sqrt{2mE}}{\hbar}$$

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

$$\psi(x) = A\sin(Kx) + B\cos(Kx) \quad \text{—— 1}$$

where A and B are constants determined by boundary conditions.

$\therefore$ at $x = 0$ and $x = L$ we get

$\psi(0) = 0$

$\psi(L) = 0.$

$\therefore$ $\psi(0) = 0$ can be substituted in general equation

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

As $\psi(0) = 0$ then $B = 0$

$\therefore$ $\psi(x) = A\sin(Kx)$

Apply $\psi(L) = 0$

$\therefore x = L$

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

Since $A \neq 0$ (otherwise, the wave function would be zero everywhere)

$$\sin(kL) = 0$$

$$kL = n\pi \quad (\because n = 1, 2, 3 \ldots)$$

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

$\therefore$ from eq (i)

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{L}$$

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

$\therefore$ The quantized energy levels of a particle in a 1D box (infinite potential well) are given by

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

where $n = 1, 2, 3 \ldots$

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Q3.) What is wave function Ψ? Write mathematical conditions of well behaved wave function.

Ans. The wave function Ψ represents the quantum state of a particle where $|\Psi(x,t)|^2$ gives the probablity density of finding the particle at postion x and time t.

Conditions for well behaved wave are as follows:-

i.) Normalization :- The wave function must be square integrable over all space, so that total probablity of finding the particle somewhere in space is 1

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

ii.) Single Valuedness :- The wave function must be single valued at each point in space $\Psi(x,t)$ is single valued for any x.

iii.) Continuity :- The wave function $\Psi(x,t)$ must be continous and smooth (differentiable) everywhere, except possibly at points where the potential $(V(x))$ is infinite

iv.) Finite amplitude :- The wave function, $\Psi(x,t)$ must be finite everywhere in space

$|\Psi(x,t)| < \infty$ for all values of x.

v.) Continous derivative :- $\frac{d\Psi}{dx}$ is continous, except at infinite potential points

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Q4.) Discuss any two applications of Tunneling effect.

Ans. The tunneling effect is a quantum phenomenon where particles can pass through a potential barrier that they classically shouldn't be able to overcome. Here are 2 applications of it:-

a.) Scanning Tunneling Microscope (STM):- STM uses electron tunneling between a sharp tip and a surface to map atomic structure with high precision.

b) Nuclear Fusion in Stars:- Tunneling allows protons to overcome repulsion barriers, enabling fusion reactions in stars like the sun and releasing energy.

Q5.) An electron is accelerated by a potential difference of 10 KV What is De Broglie associated with this electron.

Ans. Given :- potential difference (V) = 10 KV = 10 000 V

To find :- De Broglie wavelength (λ)

Solution :-

$$K.E = eV \qquad (K.E = \text{Kinetic Energy})$$

$$K.E = 1.602 \times 10^{-19} \times 10\,000$$

$$= 1.602 \times 10^{-15}\,J.$$

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

$$\therefore p = \sqrt{2mK.E}$$

$$\therefore p = \sqrt{2 \times 9.109 \times 10^{-31} \times 1.602 \times 10^{-15}}$$

$$\therefore p = 5.39 \times 10^{-24}\ kg\,m/s.$$

$$\therefore \lambda = \frac{h}{p} \quad (\text{de Broglie hypothesis})$$

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$$\lambda = \frac{6.626 \times 10^{-34}}{5.39 \times 10^{-24}}$$

$$\lambda = 1.23 \times 10^{-10} m.$$

$\therefore$ The de Broglie wavelength associated with the electron is approximately $1.23 \times 10^{-10} m$

Q6.) Explain De Broglies hypothesis in detail and hence calculate the de Broglie wavelength of a.) 1 keV electron b.) 1 keV proton and c.) 1 keV neutron

Ans de Broglie's Hypothesis states that all matter exhibits both wave-like and particle like properties, suggesting that particles such as electrons, protons and neutrons have an associated wavelength called de Broglie wavelength.

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

Given :- Energy $(E) = 1\,keV = 1.602 \times 10^{-16} J$
Mass of electron :- $m_e = 9.109 \times 10^{-31} kg$
To find :- de Broglie wavelength

$$p = \sqrt{2mKE} = \sqrt{2 \times 9.109 \times 10^{-31} \times 1.602 \times 10^{-16}}$$

$$p = 5.4 \times 10^{-24} \ kg\,m/s.$$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}}{5.4 \times 10^{-24}} = 1.23 \times 10^{-10} m.$$

$\therefore$ The de Broglie wavelength associated with electron is $1.23 \times 10^{-10} m$

1keV proton

Given :- ~~Energy~~ mass of proton $(m_p) = 1.673 \times 10^{-27}$ kg

$$p = \sqrt{2mE} = \sqrt{2 \times 1.673 \times 10^{-27} \times 1.602 \times 10^{-16}} = 7.31 \times 10^{-22}\ kg\ m/s$$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}}{7.31 \times 10^{-22}} \approx 9.06 \times 10^{-13}\ m$$

1keV neutron.

Given :- mass of neutron $(m_n) = 1.675 \times 10^{-27}$ kg

$$p = \sqrt{2mE} = \sqrt{2 \times 1.675 \times 10^{-27} \times 1.602 \times 10^{-16}} = 7.31 \times 10^{-22}\ kg\ m/s$$

$$\therefore \lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}\ Js}{7.31 \times 10^{-22}\ kg\ m/s} \approx 9.06 \times 10^{-13}\ m$$

$\therefore$ The de broglie associated with proton and neutron is 9.06×10^{-13} m.

Q7.) An electron is bound by a potential which closely approaches an infinite square well of width 1A°. Calculate the lowest two permissible energies (in electron volts) the electron can have.

Ans. Given :- width of square well $(L) = 1$ A°

To find :- Lowest two permissible energies the electron can have.

Solution :-

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

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

$$\approx \frac{1 \times 4.39 \times 10^{-68}}{7.2872 \times 10^{-50}} \approx 6.02 \times 10^{-19}\ J.$$

$\therefore$ E_1 to eV

$$E_1 \approx \frac{6.02 \times 10^{-19}\ J}{1.602 \times 10^{-19}} = 3.76\ eV \text{ —— (i)}$$

for $n=2$.

$$E_2 = \frac{(2)^2 (6.626\times10^{-34})^2}{8\times(9.109\times10^{-31})(1\times10^{-10})^2}$$

$E_2 = 4E_1$ (from (i))

$\therefore E_2 = 4\times3.76 \approx 15.04\,eV$

Thus, the lowest permissible energies for the electron are $E_1 \approx 3.76\,eV$, $E_2 \approx 15.04\,eV$.

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