Unit No-3
Quantum Physic
WAVE PARTICLE DUALITY

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Introduction

The wave theory of light successfully explained the optical phenomenon like reflection, refraction, interferences, diffraction, and polarization but it failed to explain the phenomenon of photoelectric effect and Compton Effect. These phenomena were explained on the basis of quantum theory. According to quantum theory a beam of light of a frequency ν consist of small packets each having energy $h\nu$ called photon or quanta. These photons behave like particles. Thus light possesses dual nature. Sometime it behaves like a wave and sometime like a corpuscle.i.e.Particle.

In short, to explain the photoelectric effect and Compton Effect we must treat electromagnetic radiation as particle. Even though it is essential to assign both wave and particle aspect to electromagnetic radiation, in any experimental situation one model can be applied. Never both! Accordingly, In 1928 Neil Bohr started the principle of complementarily. The wave and particle aspects of electromagnetic radiation are complementarily. Bohr's principle of complementarily is applicable to the dual nature wave and particle of material particles such as electrons, photons and others. The measurement of e/m and other characteristics of cathode ray clearly established the particle aspects of the electrons.

Whereas electrons or any other material particles must be assigned wave of de-Broglie wavelength in order to explain the diffraction of material particles. When we speak of photons we know that it is the electromagnetic wave that is associated with them. In case of material particles, we know their wavelength from the de-Broglie hypothesis, but we do not know the nature of these waves. The wave, which guide the motion of particles, are called **Matter wave.**

De Broglie Hypothesis

According to de Broglie, a moving particle whatever its nature, has wave associated with it. De Broglie postulated that a free particle with rest mass 'm' moving with non-relativistic speed 'v' has a wave associated with it. The wavelength λ of such a wave is given by

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

where 'h' is Plank's constant.

De Broglie Wavelength by Analogy with Radiation

By Planck's quantum theory of radiation, the energy of a photon is given by,

$$E = h\upsilon \qquad \text{.......(1)}$$

where h is Planck's constant and ν is the frequency of radiation.
According to Einstein's theory of relativity,

$$E = mc^2 \qquad \text{.......(2)}$$

where E is the energy equivalence of mass 'm' and c is the velocity of light.

From equations (1) and (2), we have

$$h\upsilon = mc^2$$

But $$\upsilon = \frac{c}{\lambda}$$

$\therefore$ $$\frac{hc}{\lambda} = mc^2$$

$\therefore$ $$\lambda = \frac{h}{mc} \qquad \text{.......(3)}$$

If p is the momentum of a photon, then

$$p = mc$$

From equation (3), we get,

$$\lambda = \frac{h}{p} \qquad \text{.......(4)}$$

De Broglie carried these consideration over to the dynamics of a particle, and said that the wavelength λ of the wave associated with a moving particle having a momentum mv is given by

$$\lambda = \frac{h}{mv} = \frac{h}{p} \qquad \text{.......(5)}$$

From above equation (5) we see that the wavelength of radiation is related to the momentum of photon through plank constant. **De-Brogile put forward an outstanding idea in 1924 that nature must have a fundamental symmetry and hence above equation (5) must be true for photon as well as material particle**.

Question: **State de-Broglie hypothesis**	**(2M)**

De Broglie Wavelength in terms of Kinetic Energy

If the particle of mass 'm' is moving with speed 'v', its kinetic energy is given by,

$$E = \frac{1}{2}mv^2 \qquad \text{.......(1)}$$

or $$E = \frac{1}{2m}m^2v^2$$

or $$E = \frac{p^2}{2m} \qquad (\because p = mv)$$

$\therefore$ $$p^2 = 2mE$$

$\therefore$

$\therefore$ $$p = \sqrt{2mE} \qquad \text{.......(2)}$$

The de Broglie wavelength associated with a moving particle is given by

$$\lambda = \frac{h}{p} = \frac{h}{mv} \qquad \text{.......(3)}$$

From (2) and (3), we get,

$$\lambda = \frac{h}{\sqrt{2mE}} \qquad \text{.......(3)}$$

De-Broglie Wavelength of an Electron

If a charged particle say an electron is accelerated through a potential difference of V volts then the kinetic energy of the electron is

$$E = eV \qquad \text{.......(1)}$$

The wavelength of an electron in terms of kinetic energy is

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

or

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

If m_o is the rest mass of electron, then

$$\lambda = \frac{h}{\sqrt{2m_o eV}} \qquad \text{.......(2)}$$

Now,

$h = 6.625 \times 10^{-34}$ Js
$m_o = 9.1 \times 10^{-31}$ Kg
$e = 1.6 \times 10^{-19}$ C

Hence, putting these values in equation (2), we get,

$$\lambda = \frac{12.26}{\sqrt{V}} A^\circ \qquad \text{.......(3)}$$

Question:

1. State de-Broglie hypothesis of Matter wave. Show that de-Broglie wavelength of a charged particle is inversely proportional to the square root of the accelerating potential. (6M)

2. State de-Broglie hypothesis of Matter wave. Derive an expression for de-Broglie wavelength in term of Kinetic Energy. (6M)

CONCEPT OF PHASE VELOCITY AND GROUP VELOCITY

Phase Velocity

The speed with which the phase (a crest or a trough) of a wave, is propagate called the **phase velocity** of de Broglie waves. It is also known as **wave velocity** v_p

or

A single (infinite) wave is described by the expression $\sin\left[\left(\frac{2\pi}{\lambda}(x-Vt)\right)\right]$ or $\cos(wt-kx)$ or equivalent. The pattern travels with a velocity is called Phase or Wave velocity.

A particle of mass 'm' moving with velocity 'v' has a wave associated with it given by

$$\lambda = \frac{h}{mv} \qquad \text{.......(1)}$$

Let E be the total energy of the particle, and ν be the frequency of the associated wave. Equating the quantum expression E = hν with the relativistic formula for total energy, we get,

$$h\upsilon = mc^2$$

or

$$\upsilon = \frac{mc^2}{h} \qquad \text{.......(2)}$$

The equation of a plane wave of frequency ν and wavelength λ in the positive x direction is given by

$$y = a\sin(\omega t - kx)$$

where

$$\omega = 2\pi\upsilon \ \text{x} \ \frac{\lambda}{2\pi}$$

The wave moves with a phase velocity,

$$v_p = \frac{\omega}{k} \qquad \text{.......(3)}$$

Putting the values of ω and k in equation(3), we get

$$v_p = 2\pi\upsilon \ \text{x} \ \frac{\lambda}{2\pi}$$

or

$$v_p = \upsilon\lambda \qquad \text{.......(4)}$$

Substituting equations (1) and (2) in equations (4), we get

$$v_p = \frac{mc^2}{h} \ \text{x} \ \frac{h}{mV}$$

or

$$v_p = \frac{c^2}{V} \qquad \text{.......(4)}$$

For any particle V is less than C, the speed of light, we see that the phase speed comes to be greater than C! Which is an unexpected result? Another argument is that, if de-Broglie wave is associated with a moving a particle then wave must have speed same as that of a particle. Thus we have the inadequacy in equation (4) to represent a wave associated with a material particle. The difficulty raised above can be overcome by understanding the wave group and group velocity.

We can represent a wave in a simple form

$$Y = a.\sin\left(2\pi.\nu.t - \frac{2\pi.\nu.X}{V_P}\right) \quad \text{--(5)}$$

$$but$$

$$V_P = \nu.\lambda$$

$$\frac{\nu}{V_P} = \frac{1}{\lambda}$$

Equation (5) become

$$Y = a.\sin\left(2\pi.\nu.t - \frac{2\pi.X}{\lambda}\right) \quad \text{-----------------------------(6)}$$

We have two important quantity

Angular frequency $W = 2.\pi.\nu$ ---------------------(7)

Propagation constant $K = \dfrac{2\pi}{\lambda}$ ---------------(8)

From (7) and (8) Equation (6) become

$$Y = a.\sin(wt - kx) \text{-------------------------(9)}$$

from (7) and (8)

$$\nu = \frac{w}{2\pi} \quad \text{and} \quad \lambda = \frac{2\pi}{k}$$

$$V_P = \nu.\lambda = \frac{w}{2\pi} \times \frac{2\pi}{K} = \frac{w}{K} \text{--------------------}\mathbf{(10)}$$

We encounter two difficulties with equation (10). One of the features that distinguish a wave from a particle is that a wave has continuity in space and hence is unlocalised i.e. it is spread out, while material particle is always localized. Therefore if a wave given by equation (10) is associated with a moving body then probability density $\psi\psi^*$ will be proportional to a^2 which is constant. But this is not correct. Because if a body of finite size moves with a velocity V then probability of finding it at a given instant maximum at its center of mass and probability should rapidly deceases on both side of the center of mass. Such wave can be shown as in fig (1). Which is called a wave group or wave packet? Wave packet is obtained by combing many waves of different frequencies and amplitude so that resultant has a high value of amplitude near the vicinity of the particle and zero elsewhere.

Group Velocity

Superposition of waves having slightly different frequencies and amplitudes gives rise to a **wave packet** or a **wave group**. The velocity with which a wave group travels is called the **group velocity v_g.**

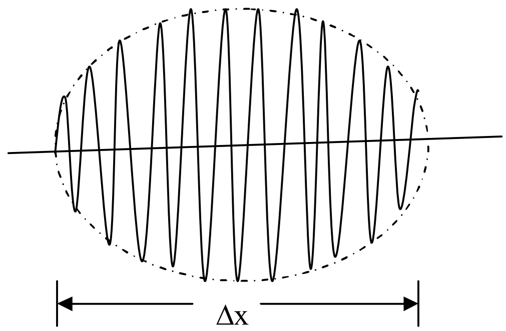


Fig. 1: Wave packet

Consider a wave packet formed by superposition of two waves of equal amplitude A with different angular frequencies and propagation constants.
Let the two waves be,

$$y_1 = A \sin(\omega_1 t - k_1 x) \qquad ....(1)$$

and

$$y_2 = A \sin(\omega_2 t - k_2 x) \qquad ....(2)$$

The resultant displacement y at any time 't' and any position x is given by

$$y = y_1 + y_2$$
$$= A [\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)]$$

$$y = 2A\cos\left[\left(\frac{\omega_1 - \omega_2}{2}\right)t - \left(\frac{k_1 - k_2}{2}\right)x\right]\sin\left[\left(\frac{\omega_1 + \omega_2}{2}\right)t - \left(\frac{k_1 + k_2}{2}\right)x\right] \qquad ....(3)$$

$$\because \sin A + \sin B = 2\sin\frac{A+B}{2}\cos\frac{A-B}{2}$$

Comparing this equation with the standard wave displacement equation,

$$y = A\sin(\omega t - kx),$$

the resultant amplitude is

$$A = 2a\cos\left[\left(\frac{\omega_1 - \omega_2}{2}\right)t - \left(\frac{k_1 - k_2}{2}\right)x\right]$$

and the angular frequency is $\left(\frac{\omega_1 + \omega_2}{2}\right)$.

The amplitude of the wave group is modulated both in space and time. Hence the velocity of the wave group v_g is given by

$$v_g = \frac{\omega_1 - \omega_2}{k_1 - k_2} = \frac{d\omega}{dk} \qquad ....(4)$$

This is the expression for the **group velocity.**

To show that group velocity v_g is equal to particle velocity v.

Consider a particle of mass 'm' moving with velocity 'v' whose kinetic energy is given by

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} \qquad (\because p = mv) \ldots\ldots.(1)$$

Also $\quad E = h\upsilon$

or $\quad E = \hbar\,\omega \qquad \left(\because \omega = 2\pi\upsilon \text{ and } \hbar = \frac{h}{2\pi}\right) \ldots\ldots.(2)$

The de Broglie wavelength is given by,

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

$$\therefore \quad p = \frac{h}{\lambda} = \frac{h}{2\pi} x \frac{2\pi}{\lambda}$$

$$\therefore \quad p = \hbar k \qquad \ldots\ldots.(3)$$

Using equations (2) and (3) in equations (1), we get

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

$$\therefore \quad \hbar\,\omega = \frac{\hbar^2 k^2}{2m}$$

$$\therefore \quad \omega = \frac{\hbar k^2}{2m}$$

Differentiating, we get,

$$d\omega = \frac{\hbar k dk}{m}$$

$$\therefore \quad \frac{d\omega}{dk} = \frac{\hbar k}{m} \qquad \ldots\ldots.(4)$$

But $\quad v_g = \dfrac{d\omega}{dk}$

$$\therefore \quad v_g = \frac{\hbar k}{m}$$

or $\quad v_g = \dfrac{p}{m} \qquad \{\because p = \hbar k\}$

$$\therefore \quad v_g = \frac{mv}{m}$$

$$\therefore \quad v_g = v \qquad \ldots\ldots.(5)$$

Thus, group velocity v_g is equal to the particle velocity.

Question:

1. What is the difference between Phase Velocity and Group Velocity? Show that de-Broglie wave group associated with a moving particle travels with the same velocity as the particle. (6M)

2. Explain group velocity and Phase Velocity. Derive expression for group velocity with which a wave group travels? (6M)

PROPERTIES OF MATTER WAVES

The properties of matter waves are stated as

(1) Lighter is the particle, greater is the wavelength associated with it, since

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

(2) Smaller is the velocity of the particle, greater is the wavelength.

(3) When velocity is zero, $\lambda = \infty$, i.e. wave becomes indeterminate and it implies that matter waves are produced by moving particles. But for $v = \infty$, λ becomes zero.

(4) The velocity of matter waves is greater than that velocity of light since

$$v_g = \frac{c^2}{v}$$

(5) The velocity of matter wave depends on the velocity of material particle and is not constant.

(6) The wave nature of matter introduces an uncertainty in its location.

Question:

1. Discuss any three properties of de-Broglie wave? (2M)

HEISENBERG'S UNCERTAINITY PRINCIPLE

Heisenberg proposed a very interesting principle of far reaching importance known as the uncertainty principle. This principle is a direct consequence of the dual nature of matter. Classically a moving particle has a definite momentum and occupies a definite position in space and it is possible to determine exactly its position and momentum simultaneously. This approximation is adequate for the objects of appreciable size, but this does not describe satisfactorily the behavior of the particle of atom ic dimensions. In wave mechanics, a particle can be described by a wave packet (fig.3), which represent all about the particle and move with group velocity. From Max born probability interpretation, the particle may be found anywhere within the wave packet. This suggests that the position of the particle is uncertain within the limits of the wave packets. Moreover, the wave packet has a velocity spread and hence there is uncertainty about the velocity or momentum of the particle. This means it is impossible to know where within the wave packet particle is and what its exact momentum is its momentum.

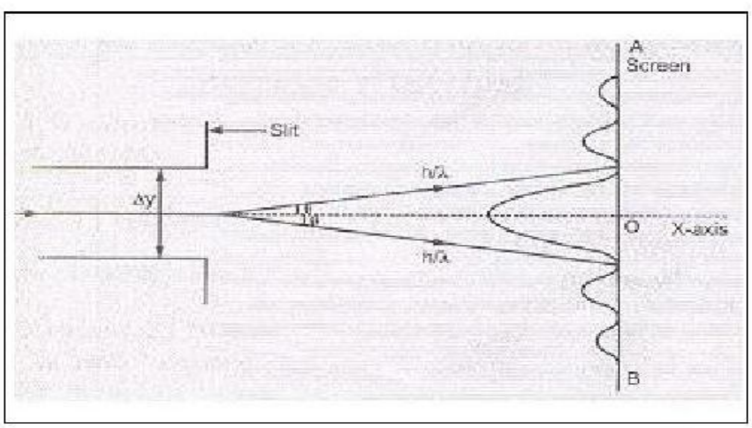
Heisenberg's uncertainty principle state that the product of uncertainties in determining the position and momentum of the particle is equal to plank's constant *h*

$$\Delta P.\Delta X = h \text{------------------} \textbf{(1)}$$

Where ΔP= uncertainty in momentum
ΔX= uncertainty in position.

ILLUSTARATION OF ELECTRON DIFFRACTIONAT A SINGLE SLIT

Consider a beam of electrons traveling towards a narrow slit a width Δy. This beam gets diffracted on passing through the slit and a diffraction pattern is obtained.



The condition for a minimum in a single slit diffraction pattern is,

$$a \sin\theta = m\lambda, \quad m = 1,2,3\ldots \qquad \ldots(1)$$

Here a is slit width and in the experiment a = slit width = Δy.

$\therefore$ Equation (1) becomes,

$$\Delta y \sin\theta = m\lambda \qquad \ldots(2)$$

$$\therefore \quad \Delta y = \frac{\lambda}{\sin\theta} \qquad (\because m = 1 \text{ for } 1^{st} \text{ minima}) \qquad \ldots(3)$$

Before entering the slit, the electrons have a definite momentum p = mv. After passing through the slit, the electrons get deflected and acquire a momentum along OA and OB.

Due to deviation in the path of electrons, the momentum of such an electron has a non-zero y component between $\frac{-h}{\lambda}\sin\theta$ and $\frac{+h}{\lambda}\sin\theta$. Thus, the uncertainty in the y components of momentum is

$$\Delta p_y = \frac{h}{\lambda}\sin\theta - \left(-\frac{h}{\lambda}\sin\theta\right).$$

$$\therefore \quad \Delta p_y = \frac{2h}{\lambda}\sin\theta \qquad \ldots(4)$$

From equations (3) and (4), we have,

$$\Delta y \,.\, \Delta p_y = \frac{\lambda}{\sin\theta} \times \frac{2h}{\lambda}\sin\theta = 2h$$

or $\Delta y \,.\, \Delta p_y \geq h$

This gives experimental support to Heisenberg's uncertainty principle.

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Questions

1. State Heisenberg's uncertainty principle and illustrate it by experiment on diffraction at a single slit.(6M)

2. What is Heisenberg's principle? Give one experiment to prove its validity.(6M)

CONCEPT OF WAVE FUNCTION & PROBABILITY INTERPRITATION

The matter wave in the form of a wave packet is represented as a function of space and time given by ψ(x,y, z, t). This is called the wave function. The value of the wave function ψ (x, y, z, t) associated with a moving particle is related to he probability of finding the particle at point (x, y, z) at time 't'.

However, ψ is usually a complex quantity. It has no direct physical significance as it is not an observable quantity. As probability is always real and positive, ψ(x, y, z, t) cannot be directly related to the probability of getting different values of a physical variable.

But the quantity $|\psi|^2$ $|\psi\psi^*|$ (where Ψ* is the complex conjugate of ψ) is a positive real number. Hence, it can be assigned some physical significance.

PHYSICAL SIGNIFICANCE OF ψ

In 1926, Max Born, a German physicist gave a physical interpretation of the wave function ψ. He suggested that $|\psi|^2 = |\psi\psi^*|$ a point (x, y, z) at time 't' gives the probability of finding the particle at that point, at that instance, in a given volume element.

If dv = dx dy dz is a small volume element surrounding the point (x,y, z), then the probability of finding the particle in that volume element is given by

$$P = |\psi|^2 dv$$

Where $|\psi|^2$ is called the **probability density.**

If the particle exists then the probability of finding the particle somewhere in space is unity.

$$\therefore \qquad \int |\psi|^2 dv = 1$$

$$\text{or} \qquad \int_{-\infty}^{+\infty} \int \int |\psi|^2 \, dx\, dy\, dz = 1 \qquad \ldots(1)$$

A wave function ψ satisfying this relation is called a **normalized wave function** and the condition is known as the **normalization condition**. The wave function ψ should satisfy the following conditions:

1. ψ should be a **normalized** wave function
2. The probability P can have only one value at a given point i.e. Ψ must be **single valued.**
3. ψ should be a **normalized** wave function.
4. ψ and its partial derivatives should be **continuous.**
5. As infinite probability has no meaning, ψ must be **finite.**

A wave function satisfying these conditions is said to be a **well behaved function.**

Question

1. Explain the physical significance of wave function ψ and ψ^2 (6M)

2. Explain the physical significance of wave function ψ and $|\psi|^2$ (6M)

SCHROEDINGER'S WAVE EQUATIONS

The mathematical representation of matter waves associated with a moving particle is known as **Schroedinger's wave equation.**

The equation is of two types:
(1) Time independent wave equation
(2) Time dependent wave equation.

Schroedinger's Time Independence Wave Equation

Consider a particle of mass 'm' moving with velocity 'v'. The position of the particle is represented by (x ,y, z) in time 't'.

According to De-Broglie's hypothesis, the wavelength of a particle associated with a wave is given by,

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

where, p = mv is the momentum of the particle.

Let, ψ(x, y, z, t) be the wave function corresponding to matter wave of a particle of mass 'm' and velocity 'v'.

The usual wave equation is Cartesian coordinates is given by

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{1}{u^2}\frac{\partial^2\psi}{\partial t^2} \qquad \ldots(1)$$

The solution of this equation is

$$\psi = \psi \circ e^{-i\omega t} \qquad \ldots(2)$$

Where $\psi \circ$ represents the amplitude of the wave associated with the moving particle.

Differentiating equation (2) twice the respect to 't', we get,

$$\frac{\partial^2\psi}{\partial t^2} = \text{-}\omega - \omega^2\psi \circ e^{-i\omega t} = \text{-}\,\omega^2\psi \qquad \ldots(3)$$

Substituting this value in equation (1),

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-\omega^2}{u^2}\psi \qquad \ldots(4)$$

Taking $\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \nabla^2\psi$

$$\therefore \qquad \nabla^2\psi = \frac{-\omega^2}{u^2}\psi$$

$$\therefore \qquad \nabla^2\psi + \frac{\omega^2}{u^2}\psi = 0 \qquad \ldots(5)$$

Here ω =2πυ and u = υλ

$$\therefore \qquad \frac{\omega^2}{u^2} = \frac{4\pi^2}{\lambda^2}$$

∴ Equations (5) becomes

$$\nabla^2\psi + \frac{4\pi^2}{\lambda^2}\psi = 0 \qquad \ldots(6)$$

or $$\nabla^2\psi + \frac{4\pi^2 p^2}{h^2}\psi = 0 \qquad \left(\because \lambda = \frac{h}{p}\right) \qquad \ldots(7)$$

The total energy E of the particle is the sum of its kinetic and potential energies.

$\therefore$ $$E = \frac{1}{2}mv^2 + V \qquad (V = P.E.)$$

or $$E = \frac{1}{2m}m^2v^2 + V$$

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

$\therefore$ $$p^2 = 2m(E - V) \qquad \ldots(8)$$

Putting value of in equation (7).

$$\therefore \nabla^2\psi + \frac{4\pi^2}{h^2} \times 2m(E - V)\,\psi = 0$$

$\therefore$ $$\nabla^2\psi + \frac{2\pi^2}{h^2}(E - V)\,\psi = 0 \qquad \ldots(9)$$

where $\hbar = \dfrac{h}{2\pi}$

Equation (9) is known as Schroedinger's time independent wave equation.

Schroedinger's Time Dependent Wave Equation

The wave function ψ is given by

$$\psi = \psi \circ e^{-i\omega t} \qquad \ldots(1)$$

Differentiating with respect to 't',

$$\frac{\partial\psi}{\partial t} = -i\omega\psi \circ e^{-i\omega t}$$

$\therefore$ $$\frac{\partial\psi}{\partial t} = -\omega\psi \qquad \ldots(2)$$

Now $\omega = 2\pi\upsilon$ and $\upsilon = \dfrac{E}{h}$

$\therefore$ $$\frac{\partial\psi}{\partial t} = -i(2\pi)\frac{E}{h}\psi$$

$\therefore$ $$E\psi = \frac{-1}{i}\left(\frac{h}{2\pi}\right)\frac{\partial\psi}{\partial t}$$

$\therefore$ $$E\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad \ldots(3)$$

where $\hbar = \dfrac{h}{2\pi}$

Schroedinher's time independent wave equation is

$\therefore$ $$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\,\psi = 0 \qquad \ldots(4)$$

Putting value of $E\psi$ in equation (4),

$$\nabla^2\psi + \frac{2m}{\hbar^2}\left(i\hbar\frac{\partial\psi}{\partial t}\right) + V\psi = 0$$

Multiplying both sides by $\frac{-\hbar^2}{2m}$, we have,

$$\frac{-\hbar^2}{2m}\nabla^2\psi - i\hbar\frac{\partial\psi}{\partial t} + V\psi = 0$$

$$\therefore \boxed{\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}} \qquad \ldots(5)$$

This equation is known as Schroedinger's time dependent wave equation.

Questions

1. Derive Schrödinger's time independent wave equation. (6M)

2. State Schrödinger's time independent and time dependent equations and state any one difference between them. What are the basic requirements for solution of the Schrödinger's equation to be acceptable? (6M)

APPLICATIONS OF SCHROEDINGER'S TIME INDEPENDENT WAVE EQUATION

Particle in a Rigid Box (infinite Potential Well)

Consider a quantum particle confined in a one-dimensional region of space between x = 0 and x = L. This particle is trapped in this box bounded by infinitely rigid walls. Such a box is called a **rigid box** or an **infinite potential well.**

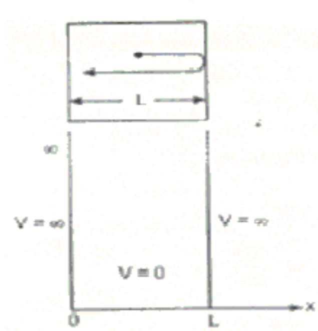


Figure 1. Infinite potential well

Classical Predictions:

- The particle can have any energy including zero.
- In probability of finding the particle anywhere in the box is equal.

The potential energy V of the particle is infinite on both sides of the box. The potential energy V can be assumed to be zero inside the box.

Thus, $V = 0$ for $0 < x < L$

$V = \infty$ for $x \le 0$ and $x \ge L$

The particle cannot exist outside the box and so its wave function ψ is zero outside the box.

i.e. $\psi = 0$ for $x \le 0$ and $x \ge L$

Schroedinger's time independent equation is

$$\nabla^2\psi + \frac{2m}{h^2}(E - V)\psi = 0 \qquad \ldots(1)$$

Within the box, the equation becomes,

$$\frac{\partial^2\psi}{\partial t^2} + \frac{2m}{h^2}E\psi = 0 \qquad (\because V = 0) \qquad \ldots(2)$$

Putting $\frac{2mE}{h^2} = k^2$, the equation becomes,

$$\frac{\partial^2\psi}{\partial t^2} + k^2\psi = 0 \qquad \ldots(3)$$

The general solution for equation (3) is given by

$$\psi(x) = A \sin kx + B \cos kx \qquad \ldots(4)$$

Using the boundary conditions to find constants A and B in equations (4), we have,

$\psi = 0$ at $x = 0$

∴ $B = 0$

∴ Equation (4) is written as,

$$\psi = A \sin kx \qquad \ldots(5)$$

Also $\psi = 0$ at $x = L$

∴ $A \sin kL = 0$

As $A \neq 0$, $\sin kL = 0$

or $kL = n\pi$

$$\therefore \quad k = \frac{n\pi}{L}, \; n = 1, 2, 3, \ldots. \qquad \ldots(6)$$

Thus, $$\psi_n(x) = a \sin\left(\frac{n\pi}{L}\right)x \qquad \ldots(7)$$

and the energy of the particle is given by,

$$E_n = \frac{\hbar^2 k^2}{2m}$$

$$= \frac{k^2 h^2}{8\pi^2 m}$$

$$E_n = \frac{n^2 h^2}{8mL^2} \qquad \left(\because k = \frac{n\pi}{L}\right) \qquad \ldots(8)$$

Thus, from equation (8), it is seen that a particle inside the box can have only discrete energy values excluding zero. These are known as **energy eigen values**.

Quantum Prediction:

- The particle can take only discrete energy values given by,

$$E_n = \frac{n^2h^2}{8mL^2} \quad n = 1, 2, 3, \ldots..$$

- The lowest energy of the particle E_1 is non-zero. The energy levels of electron in a rigid box of width 1 A° are as shown in Fig. 2.

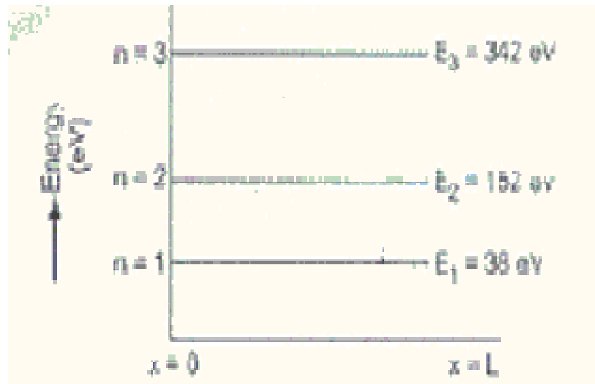


Figure 2: Energy level diagram

Wave Function of the Particle inside a Rigid Box

The wave function ψ of the particle inside the rigid box is given by,

$$\psi = A \sin kx$$

or
$$\psi = A \sin\left(\frac{n\pi x}{L}\right) \qquad \left(\because k = \frac{n\pi}{L}\right) \qquad \ldots(1)$$

The wave function ψ_n corresponding to each energy eigen value E_n is called the **eigen function.**

To evaluate the constant A in equation (1), we use the normalization condition.

$$\int_{x=0}^{x=L} |\psi_n|^2 \, dx = 1 \qquad \ldots(2)$$

$$\therefore \quad A^2 \int_{x=0}^{x=L} \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$\therefore \quad A^2 \int_{x=0}^{x=L} \left(\frac{1-\cos 2n\pi x / L}{2}\right) dx = 1$$

which gives
$$A^2 \cdot \frac{L}{2} = 1$$

∴ The normalization constant is

$$A = \sqrt{\frac{L}{2}} \qquad \ldots(3)$$

Hence the normalized wave function of the particle is given by,

$$\boxed{\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}} \qquad \ldots(4)$$

The normalized wave functions ψ_1, ψ_2, and ψ_3 and its corresponding probability densities $|\psi_1|^2, |\psi_2|^2, |\psi_3|^2$ are plotted as shown in Fig. 3 (a) and (b) respectively.

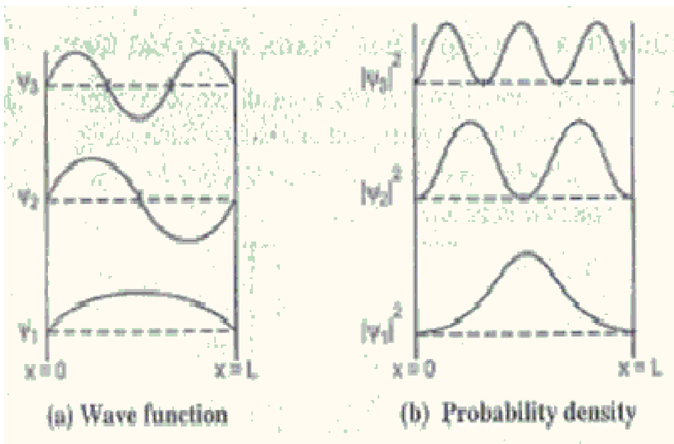


Figure.3:wave function and probability density curve.

Wave function may be negative, but $|\psi_n|^2$ is always positive. Thus, $|\psi_n|^2$ gives the probability of finding the particle at a certain place within the well.

At a particular point in the box, the probability of the particle to be present is different for different quantum numbers. For n=1, the probability density is largest in the middle i.e. at x = L/2. For n = 2, the probability density is zero at the center, but maximum at $x = \frac{L}{4}$ and $x = \frac{3L}{4}$.

Classical theory predicts the same probability for the particle to be present anywhere in the box.

Question
1. Derive an expression for the energy levels of particle enclosed within an infinite deep potential well. Show necessary waveforms. (6M) 2. Obtain an expression for energy and wave function of a particle trapped in a rigid box. (6M)

Particle in a Non-Rigid Box (Finite Potential well)

Consider a quantum particle confined in a one-dimensional region of space between x = 0 and x = L. The particle is thus trapped in a box by finite energy walls of energy V_o at x = 0 and x = L. such a box is called a non-rigid box or a finite potential well. Assume the energy E of the particle to be less than $V_{o.}$

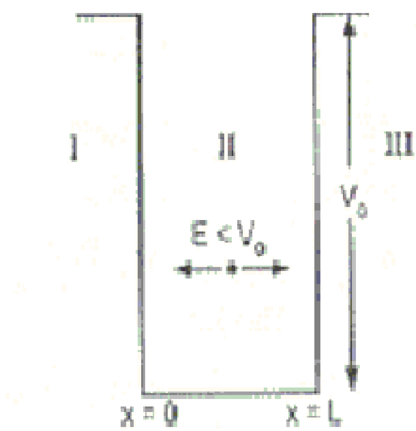


Figure 4 particle in finite potential well

Classical Prediction:

- The particle can have any energy including zero.
- The probability of finding the particle at any point inside the box is equal.
  The particle with energy E < V_o cannot exist outside the box

Schroedinger's time independent equation for a particle in one dimension is

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V)\, \psi = 0 \qquad \ldots(1)$$

Consider the three regions I, II and III separately and $\psi_{1,}$ $\psi_{2,}$ ψ_3 be the wave functions in the regions respectively.

For region I,

$$\frac{\partial^2 \psi_{I1}}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_o)\, \psi_1 = 0 \qquad (\because x \leq 0) \qquad \ldots(2)$$

For region II,

$$\frac{\partial^2 \psi_{II}}{\partial x^2} + \frac{2mE}{\hbar^2}\, \psi_{II} = 0 \qquad (\because 0 < x < L) \qquad \ldots(3)$$

For region III,

$$\frac{\partial^2 \psi_{III}}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_o)\, \psi_{III} = 0 \qquad (\because x \geq L) \qquad \ldots(4)$$

Let,

$$\frac{2mE}{\hbar^2} = k^2 \frac{2m(E - Vo)}{\hbar^2} = -k'^2 \text{ (as E < V}_o\text{)}$$

Then equations (2), (3) and (4) can be written as,

$$\frac{\partial^2 \psi_I}{\partial x^2} - k'^2 \psi_I = 0 \qquad \ldots(5)$$

$$\frac{\partial^2 \psi_{II}}{\partial x^2} + k'^2 \psi_{II} = 0 \qquad \ldots(6)$$

$$\frac{\partial^2 \psi_{III}}{\partial x^2} - k'^2 \psi_{III} = 0 \qquad \ldots(7)$$

The solutions for these equations are

$$\psi_I = Ae^{k'x} + Be^{-k'x}; \qquad x \le 0 \qquad \ldots(8)$$

$$\psi_{II} = Pe^{ikx} + Qe^{-ikx}; \qquad 0 < x < L \qquad \ldots(9)$$

$$\psi_{III} = Ce^{k'x} + De^{-k'x}; \qquad x \ge 0 \qquad \ldots(10)$$

As x $\to \pm\infty, \psi$ should not become infinite. Hence, B and C are treated as zero

B = C = 0 gives

$$\psi_I = Ae^{k'x} \qquad \ldots(11)$$

$$\psi_{II} = Pe^{ikx} + Qe^{-ikx}; \qquad 0 < x < L \qquad \ldots(12)$$

$$\psi_{III} = Ce^{k'x} + De^{-k'x}; \qquad x \ge 0 \qquad \ldots(13)$$

The constant A, P, Q, and D are determined by applying boundary conditions.

The wave function ψ and its derivative $\frac{\partial \psi}{\partial x}$ should be continuous.

$\therefore$

$$\psi_I(0) = \psi_{II}(0)$$

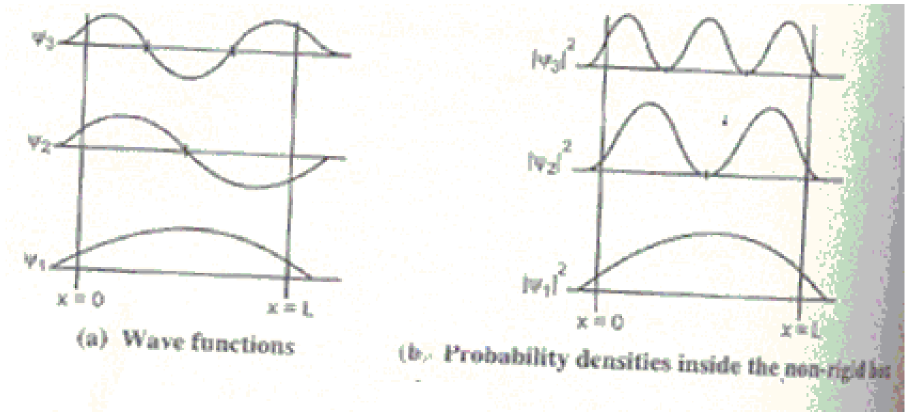
$$\left.\frac{d\psi_I}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}}{dx}\right|_{x=0}$$

$$\psi_{II}(L) = \psi_{III}(L)$$

$$\left.\frac{d\psi_{II}}{dx}\right|_{x=L} = \left.\frac{d\psi_{III}}{dx}\right|_{x=L}$$

Using these conditions, four equations are obtained from which the four constants are determined. Thus the wave functions giving complete information of particle in regions (I), (II) and (III) are obtained.

Fig. 5 (a) and (b) show the first three wave functions and probability densities plotted against x.



(a) Wave functions (b) Probability densities inside the non-rigid box

Quantum Predictions:

- The energy levels of the particle are discrete but finite.
- The lowest energy E_o is non-zero.
- Probability of finding the particle at different points in the box is different and varies with n.
- There is a small non-zero probability of finding the particle outside the box. This is called **tunneling.**

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