

4, 5, 9, 12, 13, 14, 19, 20

Unit - 2

26, 28, 29, 31, 33, 35

40, 41, 42, 46, 50

52, 54, 58, 62, 63

Quantum Mechanics

- It is a branch of physics which deals with the behaviour of matter & energy on the microscopic scale of atoms.
- The study of quantum mechanics is rooted in the early 20th century, with the pathbreaking work of Max Planck & Niels Bohr.
- Max Born coined the term quantum mechanics in 1924.
- Before 1900, most of the phenomena could be explained on the basis of the classical physics, which is based on Newton's three laws.
- Classical concepts do not hold in the region of atomic dimensions.
- Many difficulties were encountered in explaining the phenomena, which are:
 1. photoelectric effect
 2. Compton effect
 3. optical line spectra
 4. stability of atoms
 5. spectral distribution of heat radiation from black bodies.
 6. specific heats of solids at low temperature.
- The inadequacy of classical mechanics led Max Planck, in 1900 to introduce the new concept that the emission or absorption of electromagnetic radiation takes place

as discrete quanta, each of which contain an amount of energy

$$E = h\nu$$

where $h = 6.62 \times 10^{-34} \text{ J}\cdot\text{s}$ is the Planck's constant.

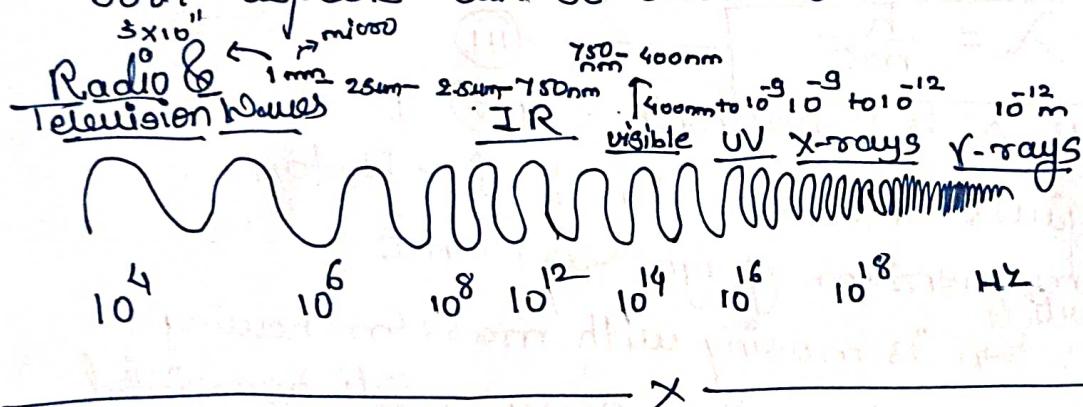
- This concept led to a new mechanism which now known as 'Quantum mechanics'.

* Wave particle duality of light *

- A Wave & particle concepts are totally based on different characteristics
- A wave is a disturbance spread out in space which is characterized by frequency, wavelength, amplitude, intensity & phase or wave velocity.
- The characteristics of a particle are its mass, velocity, & momentum & Energy.
- Though the wave & particle characteristics are totally different, certain experiments prove that radiation has dual nature, both wave-like & particle-like.
- The reason for the manifestation of wave-particle dualism can be better understood if one consider the entire Electromagnetic Spectrum.
- At the lower frequency end are radio waves whose wavelength are so large (a few hundred meters) so that an R.F (Radio frequency) wave spreads over very large volume of space.
- Therefore the energy available at any point is insignificantly small & the particle nature cannot be obtained

On the other side if UV rays or X-rays or higher frequency side of the spectrum are considered, their wavelengths are so short (few angstrom) that the wave energy is concentrated in a point of very small dimension & the wave properties are less noticeable compared to that of particle properties. Their wavelength are also short (few angstrom) i.e.

- Thus at lower frequencies the wave behaviour stands out and at higher frequencies the particle nature dominates.
- The visible region represents the transition region, where both aspects can be observed.



De-broglie hypothesis

- The idea of dualism of light was adopted by Louis de-Broglie in 1924 to all the fundamental entities.
- According to de-Broglie hypothesis every moving particle in medium is associated with wave is called matter wave or de-Broglie wave.
- According to Planck's quantum theory of photon energy is given by $E = h\nu$ ————— ① where E = Energy of photon
h = Planck's Constant
 ν = Frequency of particle

According to Einstein Energy mass relation, photon Energy is given by

$$E = mc^2 \quad \text{--- (ii)}$$

where,

m = mass of the particle

c = velocity of light

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

$$m = \frac{h\nu}{c^2} \quad (\because E = h\nu \text{ from eq (i)})$$

$$m = \frac{h\epsilon}{\lambda c^2} \quad (\because \nu = \frac{c}{\lambda})$$

$$\boxed{\lambda = \frac{h}{mc}} \quad \text{--- (iii)}$$

(where λ is wavelength of light)

\therefore This gives the wavelength for photon.

The momentum of light is $p = mc$

① Consider, an ~~electron~~^{particle} is moving with mass m , having velocity v . The momentum $mv = p$ of a particle associated with the wavelength λ is given by

$$\lambda = \frac{h}{mv} = \frac{h}{p} \quad \text{--- (iv)}$$

\therefore Equations (ii) & (iv) are de Broglie Equation.

Now, if the material particle moving with velocity v has a kinetic energy E then-

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

or

$$p = \sqrt{2mE} \quad \text{--- (v)}$$

Substituting eqⁿ ⑩ in eqⁿ ⑪, the de-Broglie wavelength of a material is -

$$\lambda = \frac{h}{\sqrt{2mE}} \longrightarrow ⑫$$

The above equation relates the wavelength of matter waves with its K.E.

- III De Broglie wavelength associated with a particle (q) accelerated by potential 'V'.

$$E = qV = eV \text{ (for Electron)}$$

$$= K.E.$$

$$K.E. = \frac{1}{2}mv^2 = qV$$

$$v^2 = \frac{2qV}{m}$$

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

Substitute above value in de Broglie eqⁿ

$$\lambda = \frac{h}{mv} = \frac{h}{m\sqrt{\frac{2qV}{m}}} = \frac{h}{\sqrt{2mqV}}$$

- IV De Broglie Wavelength for particle in thermal equilibrium at associated temp. $\rightarrow T$ then

$$E = \frac{3}{2}kT$$

$$\text{and } \lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2m\frac{3}{2}kT}} = \frac{h}{\sqrt{3mkT}}$$

where $k = 1.38 \times 10^{-23}$ Joule/kelvin is the Boltzmann's constant.

Heisenberg's uncertainty Principle

The Heisenberg's uncertainty principle states that it is impossible to know both the exact position and exact momentum of an object at the same time.

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

Explanation

- The wave nature of moving particles leads to some inevitable consequences.
 1. When a moving particle is conceptualized as a de-Broglie wave packet such as a precision becomes restricted.
 2. The particle is located in the region Δx , the linear spread of the wave packet.

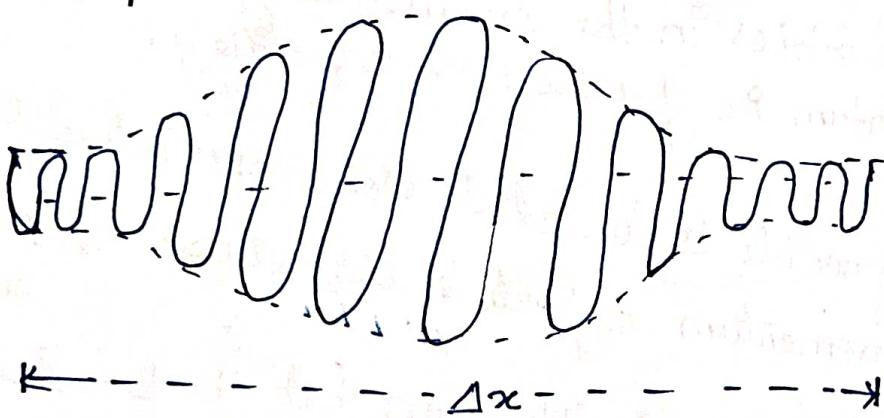


Fig. A wave packet.

- 3. The probability of finding the particle is maximum at the centre of the wave packet and falls to zero at its end. Therefore there is uncertainty Δx in the position of particle.

4. further, the wave packet is constituted by waves having a range of wavelengths, this spread in wavelength $\Delta\lambda$ is related to spread in dimension Δx :

5. As the momentum of the associated particle is related to the wavelength through the relation

$$p = \hbar k = \hbar \frac{2\pi}{\lambda} \quad (k = \frac{2\pi}{\lambda})$$

$$= \frac{\hbar}{\lambda} \cdot \frac{2\pi}{\lambda}$$

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

Their arise in uncertainty in momentum Δp .

6. The two uncertainties are inter related because the spread in momentum depends on the length of the wave packet.

spread in wavelength which is depend on the

7. The uncertainties in the knowledge of the coordinate x & momentum p_x of a $p_{x_0} + \Delta p_x$ respectively.

8. It means particle is located in somewhere between $x - \Delta x$ & $x + \Delta x$ and the momentum of particle lies between $p_x - \Delta p_x$ & $p_x + \Delta p_x$.

9. The uncertainty principle says that the product of $\Delta x \cdot \Delta p_x$ will always be greater than the value of Planck's constant.

$$\text{i.e. } \Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}$$

10. The corresponding relations for the components of position & momentum are $\Delta y \cdot \Delta p_y \geq \frac{\hbar}{2}$, $\Delta z \cdot \Delta p_z \geq \frac{\hbar}{2}$

L

Concept of Wave function (ψ)

We must consider the wave known to us such as light, sound and waves on strings etc.

- 1. Waves represents the propagation of disturbances in space.
- 2. Every wave is characterized by some quantity known as the wave variable which varies with space and time.
 - i.e. a) Sound waves have the pressure as wave variable, which varies with space and time.
 - b) Waves on strings have displacement as the wave variable
 - c) Light waves which are electromagnetic, have the field variation.
- 4. The wave variable associated with the matter wave function & it represents mathematically the motion of the particle.
The value of ψ depends on x, y, z, t
 $\therefore \psi = f(x, y, z, t)$
- 5. The value of the wave function associated with a moving body at a particular point x, y, z in space at time t is related to the likelihood of finding the body there at that time.
- 6. ψ itself has no direct physical significance & hence is not experimentally measurable.
- 7. The amplitude of the wave gives the probability of finding the particle there.

8. In general ψ is a complex valued function, we can only know the probable value in a measurement & probability can be negative.
9. ψ may be complex as,
- $$\psi = A + iB$$
- $$\psi^* = A - iB$$
- $$\therefore \psi\psi^* = A^2 + B^2 \quad (\text{which is always a real positive quantity})$$
10. Thus whether ψ is +ve or -ve or complex, the value of $|\psi|$ or $\psi\psi^*$ is always positive real number. Hence some physical meaning can be assigned to the ψ^2 or $\psi\psi^*$

Physical Significance of ψ or $|\psi|^2$

1. In 1926 Max Born gave a physical interpretation of the wave function ψ .
2. According to him $|\psi|^2$ represents the probability density. i.e. it represents the probability per unit volume of finding a particle described by the wave function ψ at a particular time t , at a particular point (x, y, z) contained in the volume.
3. A large value of $|\psi|^2$ means a strong probability of finding the particle there and a small value of $|\psi|^2$ means a little probability of its existence there.
4. $|\psi|^2 = 0$ means that the particle is absent at that point at time t .
Thus considering ψ to represent the probability density, the probability of finding the particle within a volume element, $dV = dx \cdot dy \cdot dz$ will be given by,

$$P = |\psi|^2 dV.$$
5. The total probability of finding the particle somewhere in space at all times is unity.
Hence it should satisfy the condition $\int |\psi|^2 dV = 1$

$$\int_{-\infty}^{\infty} |\psi|^2 dx dy dz = 1.$$

6. The wave function which satisfy above condition of normalization is called normalized wave function.

7. Conditions of well-behaved wave function

- I. ψ should be normalized wave function
- II. ψ should be single valued.
- III. ψ & its derivatives must be continuous everywhere in the region where ψ is defined.

Schrodinger's Wave Equation

1. Starting with De-broglie idea of matter waves, Schrodinger in 1926 developed it into mathematical theory known as a wave mechanics.
2. Schrodinger eqⁿ gives the mathematical Expressions of matter waves.
3. He argued that if De-broglie's hypothesis is correct, it should be possible to deduce the properties of an electron system from a mathematical relationship.
4. Schrodinger's equation is of two types-
 - I. Time independent Wave Equation
 - II. Time dependent Wave Equation.

Time independent Wave equation

- consider a particle of mass 'm' moving with velocity 'u'. Let (x, y, z) be the coordinate representing the positions of the particle at time 't'.

Time Independent Schrodinger's Equation

- Consider a particle of mass 'm' moving with velocity 'u'. Let (x, y, z) be the coordinates representing the position of the particle at time 't'.
- Let ψ be the wave variable associated with the matter waves. ψ is function of x, y, z & t .
- We can write the differential equation for the matter waves with wave velocity u as

$$\frac{\partial^2 \psi}{\partial t^2} = u^2 \nabla^2 \psi \quad \text{--- (1)}$$

- $\frac{\partial^2 \psi}{\partial t^2} = u^2 \nabla^2 \psi \quad \text{--- (1)}$

where $(\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$

The sol'n of eqn (1) gives us

$$\psi(x, y, z, t) = \psi_0(x, y, z) e^{-i\omega t} \quad \text{--- (2)}$$

[Where $\psi_0(x, y, z)$ is the amplitude of the wave at point (x, y, z)]

$$\therefore \psi(\vec{r}, t) = \psi_0(\vec{r}) e^{-i\omega t} \quad \text{--- (3)}$$

(Where $\vec{r} = i\hat{x} + j\hat{y} + k\hat{z}$ position vector)

Differentiating eqn (3) w.r.t 't', we get,

$$\frac{\partial \psi}{\partial t} = -i\omega \psi_0 e^{-i\omega t} \quad (\text{further differentiating})$$

$$\frac{\partial^2 \psi}{\partial t^2} = i^2 \omega^2 \psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi(\vec{r}, t) \quad \text{--- (4)}$$

from eqn (1) & (4)

$$u^2 \nabla^2 \psi = -\omega^2 \psi(\vec{r}, t)$$

$$u^2 \nabla^2 \psi + \omega^2 \psi = 0$$

Divide by u^2

$$\nabla^2 \psi + \left(\frac{\omega^2}{u^2}\right) \psi = 0 \quad \text{--- (5)}$$

we know that

$$\omega = 2\pi\nu \quad \& \quad u = v\lambda$$

where v - frequency
 u - velocity

$$\frac{\omega}{u} = \frac{2\pi\nu}{v\lambda} = \frac{2\pi}{\lambda}$$

Eqⁿ ⑤ becomes,

$$\nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi = 0 \quad \textcircled{6}$$

But de-broglie wavelength of the particle is given by,

$$\lambda = \frac{h}{p} \quad (\text{put this value in eq } \textcircled{6})$$

$$\therefore \nabla^2 \psi + \left(\frac{4\pi^2 p^2}{h^2} \right) \cdot \psi = 0 \quad \textcircled{7}$$

The total Energy of particle is

$$E = KE + P.E$$

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

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

$$E - V = \frac{p^2}{2m} \quad \text{or} \quad 2m(E - V) = p^2 \quad \textcircled{8}$$

Putting this value of p^2 in eq $\textcircled{7}$

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

$$\boxed{\nabla^2 \psi + \frac{2m}{h^2} (E - V) \psi = 0} \quad \textcircled{9} \quad \therefore \frac{h}{2\pi} = \hbar$$

This is Schrodinger's time independent equation. It is also known as Steady state of Schrodinger eq.

Schrodinger Time Dependent Wave Equation.

- Consider a particle of mass 'm' moving with velocity \vec{v} . Let (x, y, z) be the coordinates representing the position of the particle at time 't'.
- Let ψ be the wave variable associated with the matter waves. ψ is a function of $x, y, z \& t$.
- We can write the differential eqⁿ for the matter waves with wave velocity w as.

$$\frac{\partial^2 \psi}{\partial t^2} = w^2 \nabla^2 \psi \dots \dots \textcircled{1}$$

The soluⁿ of the eqⁿ ① can be,

$$\psi(x, y, z, t) = \psi_0(x, y, z) e^{-iwt} \dots \dots \textcircled{2}$$

where $\psi_0(x, y, z)$ is the amplitude of the wave

We can write eqⁿ ② as

$$\psi(x, t) = \psi_0(x) e^{-iwt} \dots \dots \textcircled{3}$$

on differentiating above eqⁿ w.r.t. to 't'

$$\frac{\partial \psi}{\partial t} = -iw \psi_0(x) e^{-iwt}$$

$$\frac{\partial \psi}{\partial t} = -i\omega \psi \dots \dots \textcircled{4}$$

$$\text{Now } \omega = 2\pi\nu \text{ & } E = h\nu$$

$$\omega = \frac{2\pi E}{h} \quad \nu = \frac{E}{h}$$

$$\frac{E}{2\pi} = \frac{E}{\hbar} \quad \therefore \hbar = \frac{h}{2\pi}$$

$$\omega = \frac{E}{\hbar} \quad \text{put this value of } \omega \text{ in eq } \textcircled{4}$$

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

Multiply both the sides by i

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

$$E\psi = i\hbar \frac{\partial \psi}{\partial t} \quad \text{--- (5)}$$

But we know that, Schrodinger's time independent eqⁿ is,

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

Put eqⁿ (5) in above eqⁿ we get

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

Multiply both the sides by $\frac{-\hbar^2}{2m}$, we get

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

This equation is Time dependent Wave equation.

Application of Schrodinger's Time Independent Wave Equation.

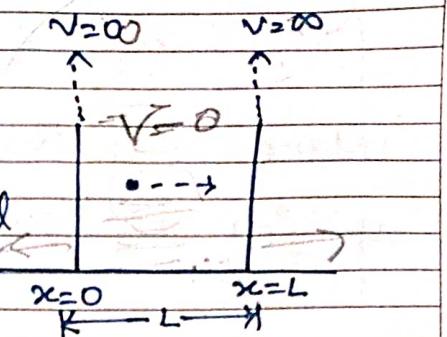
- In a wave mechanics a moving particle is associated with a wave system and the wave function ψ gives description of the system.
- Schrodinger's time independent wave eqⁿ when applied to a system determines the possible wave function.
- It can also determine the possible energy states.
- We discuss the soluⁿ of Schrodinger eqⁿ when applied to
 - Particle in rigid box.
 - Particle in non-rigid box.

Particle in a Rigid-Box

(Infinite Potential Well)

1. Consider, a particle of mass 'm' moving with velocity 'v' along the x-direction.

2. Let its motion is restricted between $x=0$ and $x=L$ inside a box bounded by infinitely rigid box.



3. The potential Energy of a particle is infinite outside the box. And is constant inside the box.

4. For convenience, suppose that the P.E $v=0$ inside the box. Thus we have,

$$V(x) = \infty \text{ for } x \leq 0 \text{ and } x \geq L$$

$$V(x) = 0 \text{ for } 0 < x < L$$

5. Let ψ be the wave function associated with the particle inside the box.

6. The particle can not have infinite amount of energy. It can not exist outside the box. Hence its wave is zero outside the box.

7. We shall apply Schrodinger Time independent wave equation to get Energy of the particle,

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - v) \psi = 0 \quad \text{--- (1)}$$

$v=0$ inside the box and particle moves along x-direction only.

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E) \psi = 0 \quad \text{--- (2)}$$

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

$$\therefore \frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad \text{--- (3)}$$

The general soluⁿ of the above differential equation is,

$$\psi(x) = A \sin(kx) + B \cos(kx) \quad \text{--- (4)}$$

where A & B are constants & can be determined by applying the boundary conditions.

The particle have boundary conditions,

$$\psi=0 \text{ at } x=0 \text{ put these values in eq (4)}$$

\therefore eqⁿ (4) becomes,

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

$$\therefore B = 0 + B \cdot 1$$

$$\boxed{\therefore B = 0}$$

\therefore eqⁿ (4) can be written as,

$$\psi(x) = A \sin kx \quad \text{--- (5)}$$

Now, Putting second condition $\psi=0$ at $x=L$ in eqⁿ (5)

$$\therefore 0 = A \sin kL$$

$A \neq 0$ since $\psi=0$ always

$$\sin kL = 0 \quad \text{i.e. } KL = n\pi$$

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

$$\therefore k^2 = \frac{n^2 \pi^2}{L^2} \quad \text{also } k^2 = \frac{2mE}{\hbar^2}$$

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

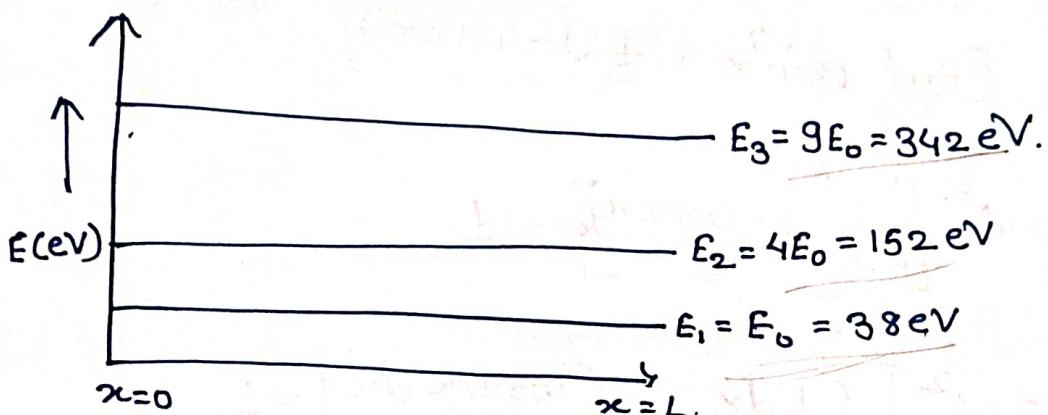
$$\boxed{E_n = \frac{n^2 \pi^2 \hbar^2}{2m L^2}}$$

$$\begin{array}{ll} E_1 & n=1 \\ E_2 & n=2 \\ E_3 & n=3 \end{array}$$

Thus the particle inside an infinite potential well can have only discrete values of Energy Excluding zero.

These are known as Energy Eigen Values of n^{th} particle.

The integer 'n' corresponding to Energy E_n is called the quantum number and it can have values. $n = 1, 2, 3, \dots$.



Wave Function of Particle Inside A rigid Box.

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

$$\psi = A \sin kx$$

$$\therefore \psi = A \sin \left(\frac{n\pi}{L} x \right) \quad \because (k = \frac{n\pi}{L})$$

$$\therefore \psi = A \sin \left(\sqrt{\frac{2mE}{\hbar^2}} x \right) \quad \because k^2 = \frac{2mE}{\hbar^2}$$

- Corresponding to Each Energy Eigen Value ' E_n ', we have the Wave function Ψ_n .
- These are known as Eigen functions of the particle
- For Ψ_n to be normalized Wave function it must satisfy the Condition,

$$\int_{x=0}^{x=L} |\psi_n|^2 dx = 1$$

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

$$[\text{Put } \sin^2 x = \frac{1}{2}(1 - \cos 2x)]$$

$$\therefore A^2 \left[\int_0^L \frac{1 - \cos 2x}{2} dx \right] = 1$$

$$\therefore A^2 \left[\int_0^L \frac{1}{2} dx - \int_0^L \frac{\cos 2x}{2} dx \right] = 1$$

$$\therefore A^2 \cdot \left[\frac{L}{2} - 0 \right] = 1$$

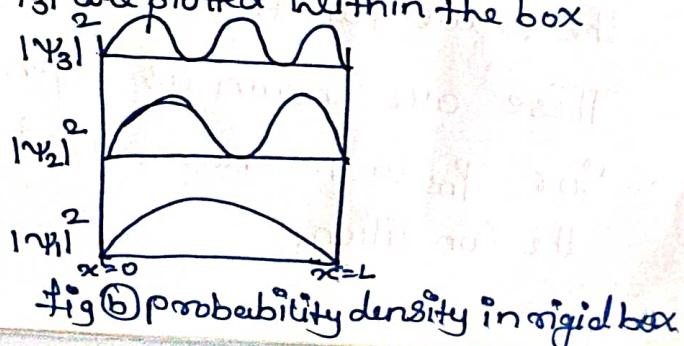
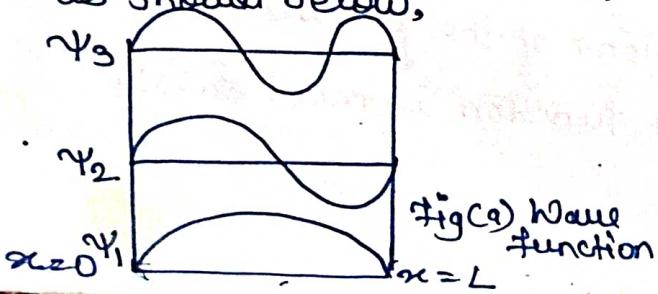
$$\therefore A^2 \cdot \frac{L}{2} = 1$$

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

- Hence, the normalized wave functions of the particle will be given by.

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

- The normalized wave functions Ψ_1, Ψ_2, Ψ_3 together with the probability densities $|\Psi_1|^2, |\Psi_2|^2$ & $|\Psi_3|^2$ are plotted within the box as shown below,



particle in a Non-rigid box

(finite potential well)

- Consider a particle of mass 'm' moving with velocity 'u' along the x-direction between $x=0$ and $x=L$

- Let E be the total Energy of particle inside the box and V be its potential energy.

- Potential Energy (V) is assumed to be zero within the box.

- The potential outside the box is finite say v_0 and $v_0 > E$

- If ψ is the wave function associated with the particle then Schrodinger time independent wave equation for it is,

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

- Consider the three regions I, II & III separately and let ψ_I, ψ_{II} & ψ_{III} be the wave function in them respectively

for region I :
$$\frac{\partial^2 \psi_I}{\partial x^2} + \frac{2m}{\hbar^2} (E - v_0) \psi_I = 0$$

for region II :
$$\frac{\partial^2 \psi_{II}}{\partial x^2} + \frac{2m}{\hbar^2} (E) \psi_{II} = 0$$

for region III :
$$\frac{\partial^2 \psi_{III}}{\partial x^2} + \frac{2m}{\hbar^2} (E - v_0) = 0$$

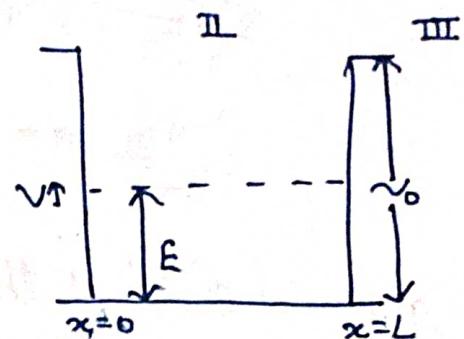


fig: finite potential well.

Let $\frac{2mE}{\hbar^2} = k^2$ and $\frac{2m(E-v_0)}{\hbar^2} = -k^2 \dots (\text{as } E < v_0)$

Then the equations in the three regions can be written as. ▼

$$\left. \begin{aligned} \frac{\partial^2 \psi_I}{\partial x^2} - k^2 \psi_I &= 0 \\ \frac{\partial^2 \psi_{II}}{\partial x^2} + k^2 \psi_{II} &= 0 \\ \frac{\partial^2 \psi_{III}}{\partial x^2} - k^2 \psi_{III} &= 0 \end{aligned} \right\} \quad (3)$$

- The general soluⁿ of these Equations are -

$$\left. \begin{aligned} \psi_I &= A e^{kx} + B e^{-kx} \quad \text{for } x < 0 \\ \psi_{II} &= P e^{ikx} + Q e^{-ikx} \quad \text{for } 0 < x < L \\ \psi_{III} &= C e^{kx} + D e^{-kx} \quad \text{for } x > L \end{aligned} \right\} \quad (4)$$

- as $x \rightarrow \pm \infty$ ψ should not become infinite.
i.e. $\psi_{II} \neq \infty$

Hence $B = 0$ & $C = 0$

Hence wave functions in three regions are -

$$\left. \begin{aligned} \psi_I &= A e^{kx} \\ \psi_{II} &= P e^{ikx} + Q e^{-ikx} \\ \psi_{III} &= D e^{-kx} \end{aligned} \right\} \quad (5)$$

- The Constants A, P, Q and D can be determined by applying the boundary conditions.
- The wave function ψ and its derivative should be continuous in the region where ψ is defined.

$$\therefore \psi_1(0) = \psi_{II}(0)$$

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

$$\frac{\partial \psi_I}{\partial x} \Big|_{x=0} = \frac{\partial \psi_{II}}{\partial x} \Big|_{x=0}$$

$$\frac{\partial \psi_{II}}{\partial x} \Big|_{x=L} = \frac{\partial \psi_{III}}{\partial x} \Big|_{x=L}$$

- using these four conditions, we get four equations to find the values of four constants A, P, Q and D.
- Thus the Wave function can be known completely
- The Eigen functions are similar in appearance to those of infinite well except that they extend a little outside the box.
- Even though the particle Energy E is less than potential Energy, there is a definite probability that the particle is found outside the box.
- The particle Energy is not enough to break through the walls of the box but it can penetrate the walls and leak out.
- This shows penetration of the particle into the classically forbidden region.

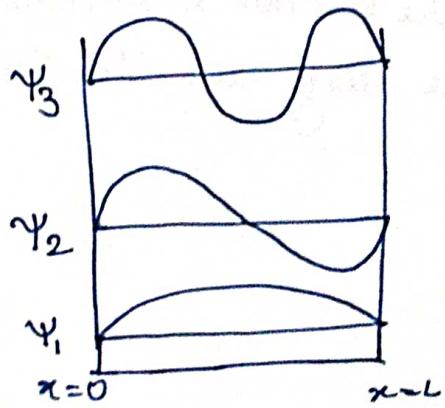


Fig @ Wave function.

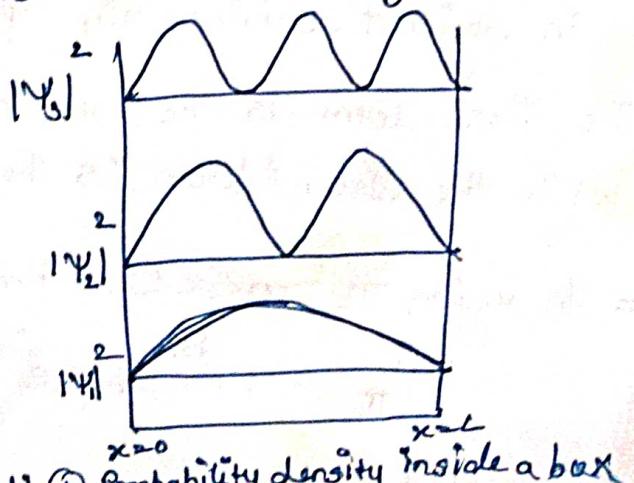


Fig (b) Probability density inside a box

Tunneling Effect

(Barrier potential)

- Consider a one dimensional Step potential as shown in Fig. Let the particle of Energy E be incident on the step from left

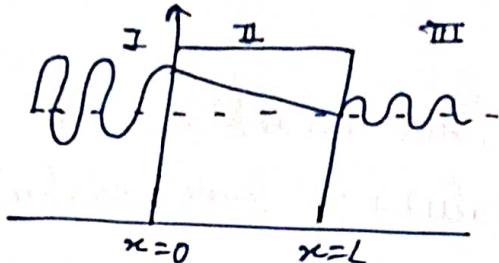
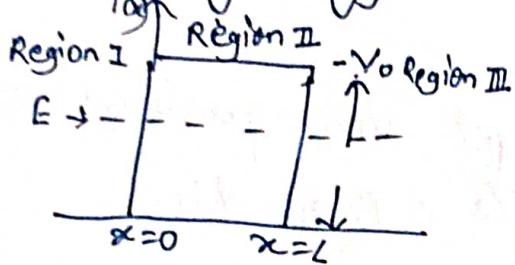


Fig ① Potential barrier of height V_0 & width L

Fig ② Potential barrier Tunnelling

- Classically we know that if $E > V_0$ the particle can enter region I, but its energy will be slowed to a value $(E - V_0)$ and it will travel with velocity $\sqrt{2(E-V_0)/m}$
- The particle thus transmitted into region III
- But if $E < V_0$ the particle can not enter region II and it reflected back into region I without the loss of speed.
- If Ψ represents the well behaved Wave Function Associated with the particle of mass 'm' and velocity v , then the Wave Function in region I, obtained as, $\Psi_I = A e^{ikx} + B e^{-ikx}$ ————— ①
- The first term is the incoming wave along the positive x-direction while the second term is the reflected wave along -ve x-direction.

= In region II : $0 < x < L$ then $V(x) = V_0$

$$\Psi_{II} = P e^{ikx} + Q e^{-ikx} \quad \text{————— ②}$$

In region III, $V_x = 0$ for $x > L$ the wave function in the region is,

$$\Psi_{\text{III}} = D e^{-k'x} \quad \textcircled{3}$$

- For determining the Constants A, B, D, P, Q the boundary conditions are applied at $x=0$ & $x=L$

$$\text{i.e. } \Psi_I = \Psi_{\text{II}} \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{at } x=0$$

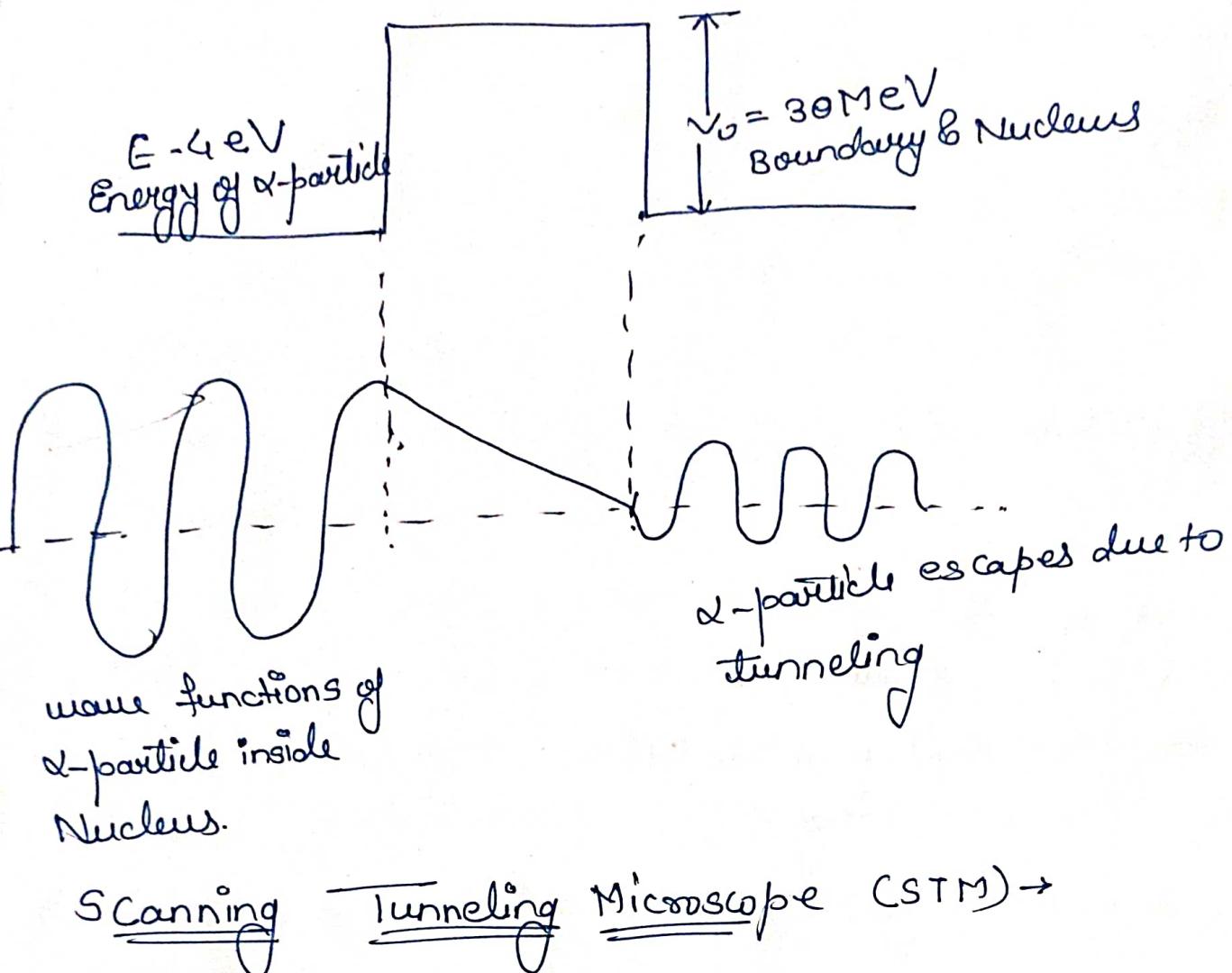
$$\frac{\partial \Psi_I}{\partial x} = \frac{\partial \Psi_{\text{II}}}{\partial x} \quad \left. \begin{array}{l} \\ \end{array} \right\}$$

$$\frac{\Psi_{\text{II}}}{\partial x} = \frac{\Psi_{\text{III}}}{\partial x} \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{at } x=L$$

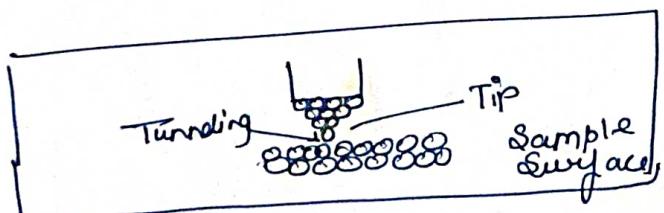
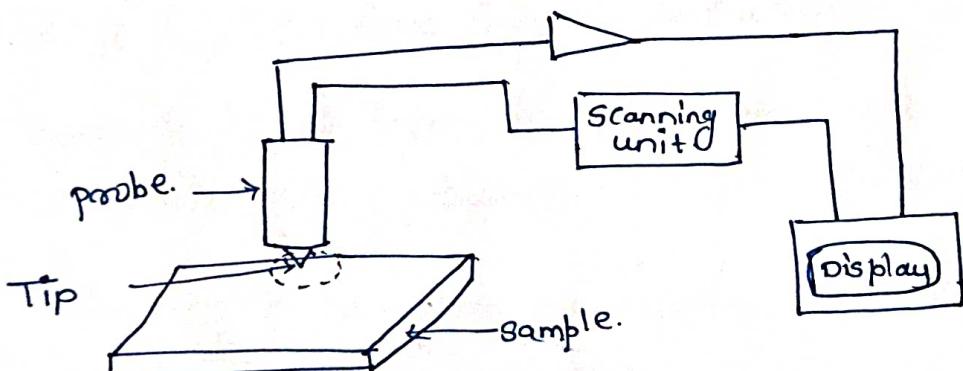
- The property of the barrier penetration is due to the wave nature of matter and is similar to the total internal reflection of light.
- The intensity of the transmitted light will decrease exponentially with the thickness of the barrier.
- If the particle incidenting on the potential barrier, there is always some probability of transmission through the barrier
- This phenomenon of crossing the barrier is called the 'Tunnelling Effect'.

Applications of Tunneling

1. α decay.
2. In α decay, an unstable nucleus disintegrates into a lighter nucleus & α -particle.
3. Uranium nucleus ^{238}U undergoes α -decay and forms thorium nucleus ^{234}Th .
4. In 1928 George Gamow Explained α -decay of unstable nuclei on the basis of quantum Tunneling.
5. The forces in the nucleus set up a potential barrier of height of the order of 30 MeV against α -particle emission.
6. According to classical mechanics, The α -particle would be trapped unless its Energy Exceeds some V.
7. The α -particle have Energies in the range of 4 to 9 MeV only.
8. Therefore it is impossible for a α -particle would be trapped unless its Energy Exceeds some V. to cross the Energy barrier.
9. According to quantum mechanics, the α -particle Tunnels through the potential barrier.



Scanning Tunneling Microscope (STM) →



1. STM Was invented by Gerd Binnig and Heinrich Rohrer Who were awarded the 1986 Nobel Prize in physics for their Work.
2. The Scanning tunneling microscope uses electron tunneling to produce images of surfaces down to the scale of individual atoms.
3. If two conducting samples are brought in close proximity with small but finite distance between them, electrons from one sample flow into the other if the distance is of the order of the spread of the electronic wave into space.
4. The probability of an electron to get through the tunneling barrier decreases exponentially with the barrier width is so called tunneling current is extremely sensitive measure of the distance between two conducting samples.

The STM Makes use of this sensitivity.

Working:-

1. In the Scanning tunneling microscope the sample is scanned by a very fine metallic tip which is connected to the scanner, an XYZ positioning device.
2. The sharp metal needle is brought close to the surface to be imaged. The distance of the order of few angstrom.
3. A bias voltage is applied between the sample & the tip.
4. When the needle is at positive potential with respect the surface, electrons can tunnel across the gap and set up a small tunnelling current in the needle. This feasible tunnelling current is amplified and measured.

5. with the help of tunneling current the feedback electronics keep the distance between tip and sample constant.
6. The sensitivity of the STM is so large that electron distribution around them can be detected.

Above fig shows the detail of set up of STM with needle tip.

