Unit 3

Quantum Mechanics

- 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,

    I) Photoelectric Effect
    II) Compton Effect
    III) Optical line spectra
    IV) Stability of atoms
    V) Spectral distribution of heat radiations from black bodies
    VI) Specific heats of solids at low temp.

- This inadequacy of classical mechanics led Max Plank in 1900 to introduce the new concepts that the emission or absorption of electromagnetic radiations takes place as descrete quanta, each of which contain an amount of energy,

$$E = h\nu$$

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

- This concepts led to ~~the~~ new mechanics which now known as 'QUANTUM MECHANICS'.

The wave particle duality of light

1. The photoeletric effect and compton effect established that light behaves as a flux of photons
2. On the other hand the phenomena of interefearence diffraction and polarisation can be explained only when light is treated as a continuous wave.
3. Neither of the model seperately explain all the experimental facts. The carpuscular nature and wave nature appear to be mutually exclusive.
4. Light behaves both as a stream of particles and as continuous wave. therefore, we say that light exhibits wave-particle duality.
5. The reason for the manifestation of wave particle dualism can be better

- understood if ~~as~~ one considers the entire electromagnetic spectrum.

6. At the lower frequency end are radio waves whose wavelengths are so large (a few hundred meters) so that an RF (Radio frequency) wave spreads over very large volume of space.

7. Therefore the energy available at any point is insignificantly small and the particle nature can not be observed.

8. On the other side, if UV or X-rays on 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 and the wave properties are less noticeable compared to that of particle properties.

9. Thus at lower frequencies the wave behaviour stands out and at higher frequency the particle nature dominates.

10. The visible region represents the transition region, where both aspects can be observed

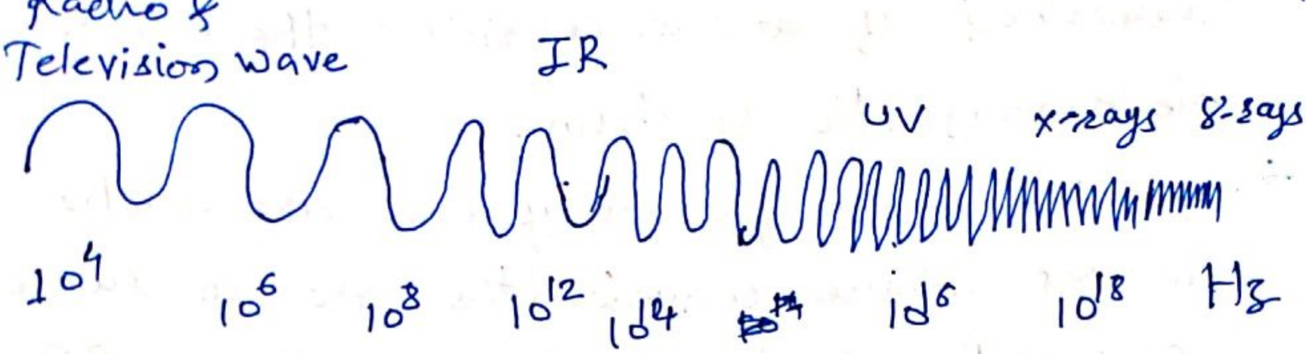

Fig. An electromagnetic Spectrum

De-Broglie's Hypothesis

1. In 1924, Louis de-Broglie, a French physist, suggested that, the wave-particle dualism need not be a special feature of light alone but the material particles must also exhibits such dual behaviour.
2. He reasoned out that since nature exhibits a great amount of symmetry, particles as well as waves exhibits - properties of both particles and waves.

   'This is known as De-Broglie's Hypothesis'
3. Accordingly, particles such as electrons, protons etc. have waves associated with them. These waves are called 'matter waves' or De-Broglie's waves'.
4. A light wave of frequency ν is associated with a photon of energy E, given by,

$$E = h\nu \quad \text{- - - - - (1)}$$

According to Einstein's theory of relativity,

$$E = mc^2$$, (where c is velocity of light)

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

$$m = \frac{h\nu}{c^2} \quad \text{- - - - (2)}$$

- Photon travels with the speed of light c hence momentum of the photon is,

$$p = mc$$

$$= \frac{h\nu}{c^2} \cdot c$$

$$p = \frac{h\nu}{c}$$

(but $\nu = \frac{c}{\lambda}$, where λ is wavelength of light.)

$$\therefore p = \frac{h}{\cancel{c}} \cdot \frac{\cancel{c}}{\lambda}$$

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

$$\text{or } \boxed{\lambda = \frac{h}{p}}$$

- Thus the wavelength associated with a photon is h/p.

- According to De-Broglie, the above eqn must be a universal relation applicable to photons as well as to any material particle.

I. A particle of mass 'm' moving with a velocity 'v' and carrying a momentum $p = mv$ must be associated with a wave of wavelength

$$\boxed{\lambda = \frac{h}{mv}}$$ De-Broglie eqn.

II. If a ~~charged~~

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

$$E = qV = eV \text{ (for electron)}$$
$$= K.E.$$

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

i.e. $E = qV$ or eV.

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

$$\therefore v = \sqrt{\frac{2qV}{m}}$$ substitute this value in De-Broglie's eqn.

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

$$\boxed{\lambda = \frac{h}{\sqrt{2mqV}}} \text{ or } \frac{h}{\sqrt{2meV}}$$

III. De-Broglie wavelength in terms of K.E.

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

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

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

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

IV. De-Broglie wavelength for particle in thermal equilibrium at associated temp 'T' then,

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

and $\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2m\frac{3}{2}KT}}$

$$\therefore \boxed{\lambda = \frac{h}{\sqrt{3mKT}}}$$

where $K = 1.38 \times 10^{-23}$ Joule / Kelvin is the Boltzman's constant.

Wave Velocity / Phase Velocity

" Defn.

When a monochromatic wave travels through a medium, its velocity of advancement in the medium is called the wave velocity."

e.g. A plane harmonic wave travelling along the +ve x direction is given by

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

where a - Amplitude

$\omega = 2\pi n$ - Angular Frequency

$K = \frac{2\pi}{\lambda}$ - Propagation constant of wave.

" The ratio of angular frequency ω to the propagation constant k is the wave velocity v_p.

i.e. $v_p = \frac{\omega}{K}$

$(\omega t - kx)$ is the phase of the wave motion.

∴ planes of constant phase are defined as

$$(\omega t - kx) = \text{constant}$$

Diff. w.r.t. t.

$$\omega - k\frac{dx}{dt} = 0$$

$$-k\frac{dx}{dt} = -\omega$$

$$\therefore v_p = \frac{dx}{dt} = \frac{\omega}{K}$$

which is the wave velocity v_p.

- Thus the wave velocity is the velocity with which planes of constant phase advance through the medium.
- Hence wave velocity is called as 'phase velocity'.

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Group Velocity (V_g).

- A pulse consists of a no. of waves differing slightly from one another in frequency.
- A superposition of these waves is called as 'wave packet' or a 'wave group'.
- When such a group travels in a medium the velocity of its different components are different.
- The observed velocity is, however, the velocity ~~wh~~ with which the maximum amplitude of the group advances in the medium, this is called a group velocity.

$$v_g = \frac{d\omega}{dk}.$$

- The group velocity is the velocity with which the energy in group is transmitted.

The Heisenberg's Uncertainty Principle

Defn - "It is not possible to make simultaneous measurements of the position and momentum of a particle to an unlimited accuracy."

$$\boxed{\Delta x . \Delta p_x \geq \frac{\hbar}{2}}$$

Explaination

- The wave nature of moving particles leads to some inevitable consequences.

1. When a moving particle is conceptualised as a de-Broglie wave packet such a precision becomes restricted.
2. The particle is located within the region Δx, the linear spread of the wave packet.

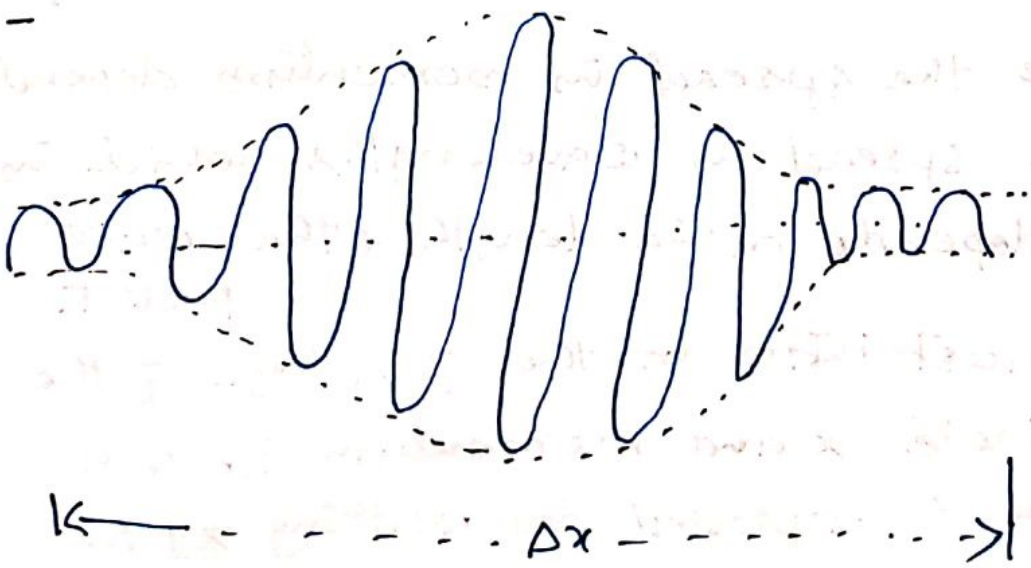


Fig. A wave Packet

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 wave lengths '$\Delta \lambda$' is related to the spread in dimension 'Δx'.

5. As the momentum of the associated particle is related to the wavelength through the relation $p = \hbar K = \hbar K \quad (K = \frac{2\pi}{\lambda})$

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

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

there arises an uncertainty in momentum Δp.

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

7. The uncertainties in the knowldge of the co-ordinate x and momentum P_x of a particle is expressed by writting $x \pm \Delta x$ and $P_x \pm \Delta P_x$ respectively.

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

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.

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

10. The corresponding relations for the other components of position and momentum are

$$\Delta y \cdot \Delta P_y \geq \frac{\hbar}{2}, \quad \Delta z \cdot \Delta P_z \geq \frac{\hbar}{2}.$$

Concept of Wavefunction (ψ)

Q. What exactly is that, which is waving in the particle wave?

1- We first consider the waves known to us, such as light, sound and waves on strings etc.

2. Waves represents the propagation of distur--bances in space.

3. Every wave is characterized by some quantity known as the wave variable which varies with space and time.

i.e. a] The 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 matter wave is called the wave function and it represents mathematically the motion of the particle.

The value of ψ depends on x, y, z & t

$$\therefore \psi \longrightarrow f(x, y, z, t)$$

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 and 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 only the probable value in a measurement & Probability can not be negative.

9. ψ May be complex as,

$$\psi = A + iB$$

$$\therefore \psi^* = A - iB$$

$$\therefore \psi\psi^* = A^2 + B^2$$ which is always a real positive quantity.

10. Thus whether ψ is +ve or -ve or complex, the value of $|\psi|^2$ or $\psi\psi^*$ is always positive real no. 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 existance there.

   $|\psi|^2 = 0$ means that the particle is absent at that point at time t.

4. 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 should satisfy the condition,

$$\int |\psi|^2 dv = 1.$$

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

6. The wave function which satisfies above condition of normalization is called normalised wave function.
7. conditions of well behaved wave function,
   I. ψ should be normalized wave function.
   II. ψ should be single valued.
   III. ψ must be finite.
   IV. ψ & its derivatives must be continuous everywhere in the region, where ψ is defined.

Schrodinger's Wave Equation

1. Starting with De-Broglie's idea of matter waves, schrodinger in 1926 developed it into mathematical theory known as a wave mechanics.
2. Schrodinger eqn gives the mathematical expression 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 systems from a mathematical relationship.
4. schrodinger's eqn is of two types,
   I. Time independent wave equation.
   II. Time dependent wave equation.

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,

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

$\left(\text{where } \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \text{ is Laplacian operator}\right)$

The solution of eqn (1) gives us,

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

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

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

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

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

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

(further differentiating)

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

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

from eqn (1) & (4)

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

$$u^2\nabla^2\psi \pm \frac{\omega^2}{\cancel{u^2}}\psi = 0 \quad \left(\text{divide by } u^2\right.$$

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

we know that,

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

where u - velocity
ν - frequancy

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

$\therefore$ eqn (5) becomes,

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

But De-Broglie wavelength of the particle is given by,

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

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

The total energy of particle is,

$$E = K.E + P.E$$

$$= \frac{1}{2}mv^2 + V$$

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

$$p^2 = 2m(E-V) \quad \cdots \quad (8)$$

putting this value of p^2 in eqn (7)

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

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

- This is schrodinger's time independent equation. it is also known as steady state of schrodinger eqn.

Schrodinger's Time Dependent Wave Equation

- consider a particle of mass 'm' moving with velocity u, let (x, y, z) be the co-ordinates 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 and t.
- We can write the differential eqn for the matter waves with wave velocity u as,

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

- The soln of eqn (1) can be,

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

where $\psi_0(x, y, z, t) = \psi_0(x, y, z)\, e^{-i\omega t}$

where $\psi_0(x, y, z, t)$ is the amplitude of the wave we can write eqn ② as,

$$\psi(r,t) = \psi_0(\bar{r}).\, e^{-i\omega t} \quad \cdots ③$$

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

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

$$\frac{\partial \psi}{\partial t} = -i\omega \psi \quad \cdots\cdots ④$$

Now, $\omega = 2\pi\nu$ and $E = h\nu$

$$= 2\pi \frac{E}{h} \qquad \nu = \frac{E}{h}$$

$$= \frac{E}{h/2\pi}$$

$\omega = \dfrac{E}{\hbar}$ put this value of ω in eqn ④

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

multiply by sides by i we have

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

$$\boxed{E\psi = i\hbar \frac{\partial \psi}{\partial t}} \quad \cdots ⑤$$

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

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

put eqn ⑤, we get

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

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

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

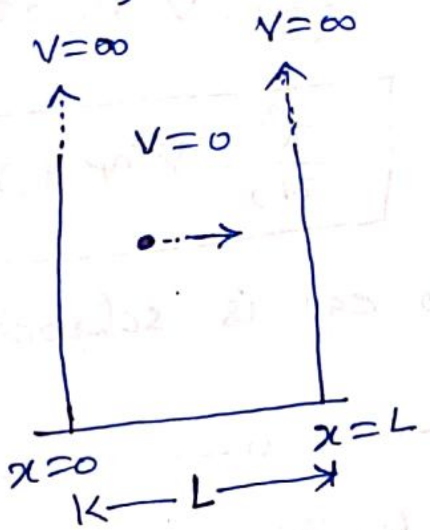
$$\boxed{\frac{-\hbar^2}{2m} \cdot \nabla^2\psi + V\psi = i\hbar \frac{\partial \psi}{\partial t}}$$

This eqn is schrodinger's 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 systems.
- 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 soln of schrodinger's eqn when applied to
  - I) Particle in rigid box.
  - II) 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 walls.

3. The potential energy of the particle is - infinite outside the box and is constant inside the box.

4. For conveinience, suppose that the P.E. [Potential Energy] $V=0$ inside the box. Thus we have,

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

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

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 S.T.I.W. eqn to get energy of the particle,

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

$V=0$ inside the box and particle moves along x-direction only,

$$\therefore \frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}\cdot E\psi = 0 \quad \cdots\cdots (2)$$

Let $\frac{2mE}{\hbar^2} = K^2$

$$\therefore \frac{\partial^2\psi}{\partial x^2} + K^2\psi = 0 \quad \cdots\cdots (3)$$

The general soln of the above differential eqn is,

$$\psi(x) = A\sin(Kx) + B\cos(Kx) \quad -- (4)$$

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

The particle have boundary conditions,

$\psi = 0$ at $x = 0$ put these values in eqn (4)

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

$\therefore$ eqn (4) becomes,

$$0 = A\sin K0 + B\cos K0$$

$$0 = 0 + B.1.$$

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

$\therefore$ eqn (4) can be written as,

$$\psi(x) = A\sin Kx \quad \cdots\cdots (5)$$

Now putting second condition eq in eqn (5)

i.e. $\psi = 0$ at $x = L$.

$$\therefore \quad 0 = A \sin KL$$

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

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

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

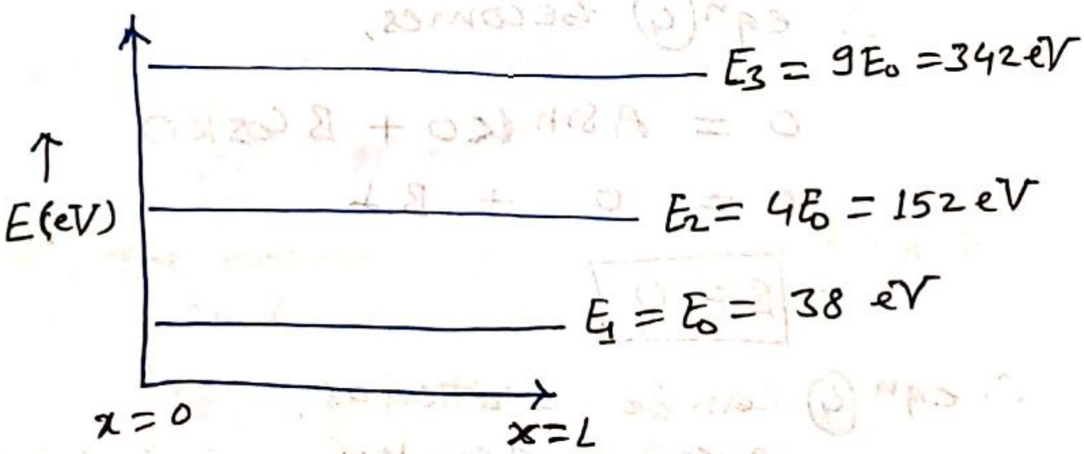
$$\therefore K = \frac{n\pi}{L}$$

$$\therefore K^2 = \frac{n^2\pi^2}{L^2} \qquad \text{Also } K^2 = \frac{2mE}{\hbar^2}$$

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

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

- 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, $n = 1, 2, 3 \cdots$



Wave function of Particle Inside A Rigid Box.

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

$$\psi = A \sin kx$$

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

$$\psi = A \sin\left(\sqrt{\frac{2mE}{\hbar^2}} \cdot x\right)$$

- 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 normalised wave function, it must satisfy the condition,

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

$$\therefore A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1. \quad \left(\text{put } \sin^2 x = \tfrac{1}{2}(1-\cos 2x)\right)$$

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

$$A^2 \cdot \frac{L}{2} - 0 = 1.$$

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

Hence, the normalised wave functions of the particle will be given by,

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

- 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,

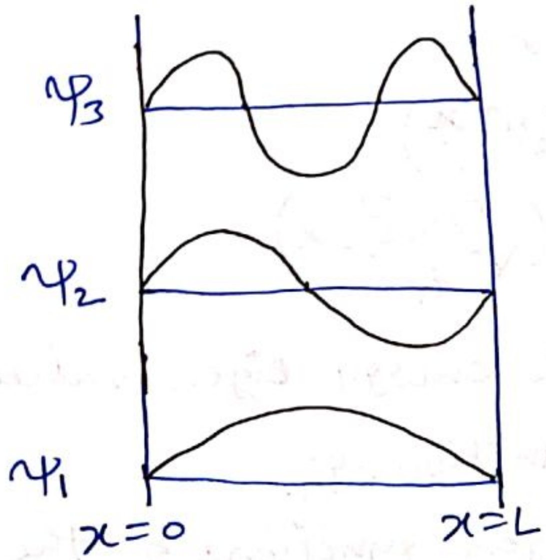


Fig. ⓐ Wave Functions

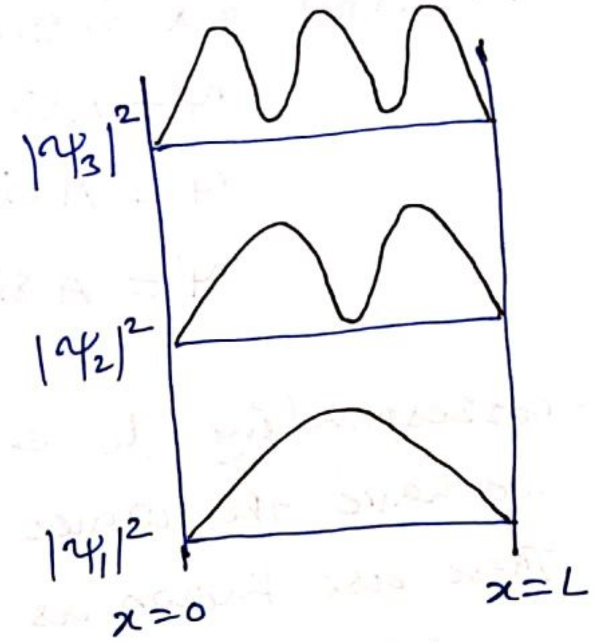


Fig ⓑ Probability density in rigid box.

Particle in a Non-rigid box.

(Infinite Potential Well)

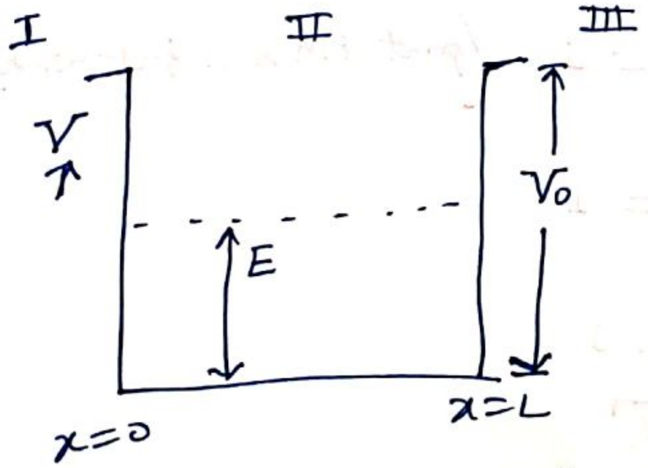


Fig: Finite Potential well.

- 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 dependent wave equation for it is,

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

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

For region I: $\quad \dfrac{\partial^2 \psi_1}{\partial x^2} + \dfrac{2m}{\hbar^2}(E-V_0)\psi_1 = 0$

For region II: $\quad \dfrac{\partial^2 \psi_{II}}{\partial x^2} + \dfrac{2m}{\hbar^2}.E\,\psi_{II} = 0$ $\quad (2)$

For region III: $\quad \dfrac{\partial^2 \psi_{III}}{\partial x^2} + \dfrac{2m}{\hbar^2}(E-V_0)\psi_{III} = 0$

Let $\dfrac{2mE}{\hbar^2} = K^2$ and $\dfrac{2m(E-V_0)}{\hbar^2} = -K'^2$ (as $E < V_0$)

- Then the equations in the three regions can be written as,

$$\left.\begin{aligned} &\frac{\partial^2 \psi_I}{\partial x^2} - K'^2\psi_1 = 0 \\ &\frac{\partial^2 \psi_{II}}{\partial x^2} + K^2\psi_{II} = 0 \\ &\frac{\partial^2 \psi_{III}}{\partial x^2} - K'^2\psi_{III} = 0 \end{aligned}\right\} \quad (3)$$

- The general sol^n of these equations are,

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

- as $x \to \pm\infty$ ψ should not become infinite.

i.e. $\psi \neq \infty$

Hence, $B=0$ and $C=0$.

Hence the wave functions in three regions are,

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

- 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.

$\therefore \psi_I(0) = \psi_{II}(0)$ $\qquad\qquad$ $\psi_{II}(L) = \psi_{III}(L)$

$$\left.\frac{\partial \psi_I}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi_{II}}{\partial x}\right|_{x=0} \qquad\qquad \left.\frac{\partial \psi_{II}}{\partial x}\right|_{x=L} = \left.\frac{\partial \psi_{III}}{\partial x}\right|_{x=L}$$

- Using these four conditions, we get four eqns to find the values of four constants A, P, Q & D.
- Thus the wave functions 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.
- Eventhough the particle energy E is less than potential energy V_0, 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.

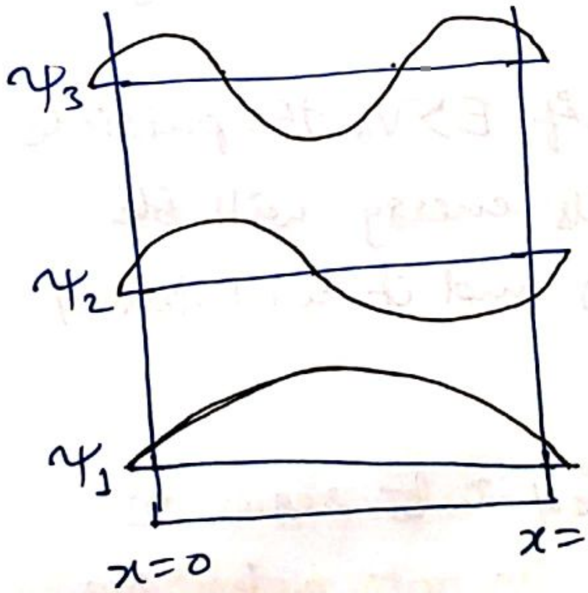


Fig ⓐ Wave function

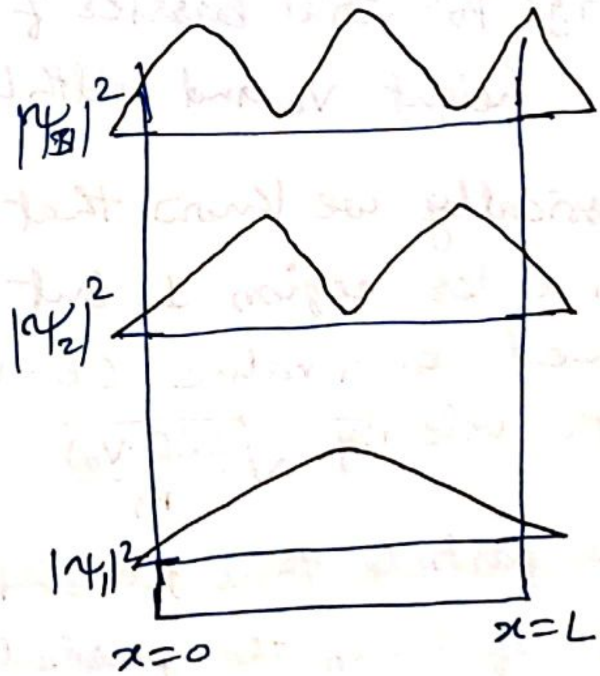


Fig. ⓑ Probability density inside rigid box.

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.

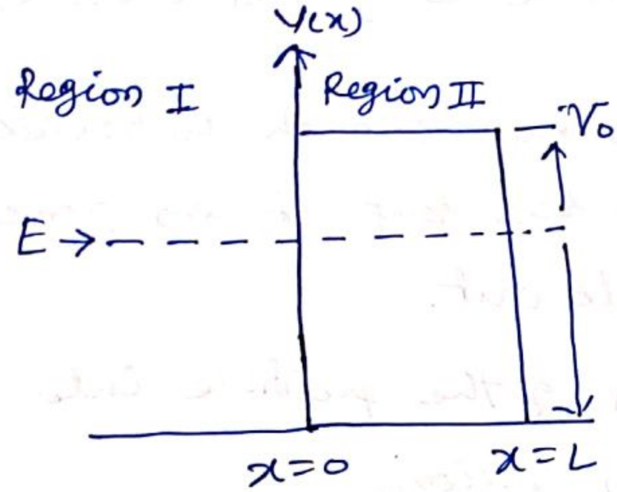


Fig: Potential barrier of height V_0 and width L.

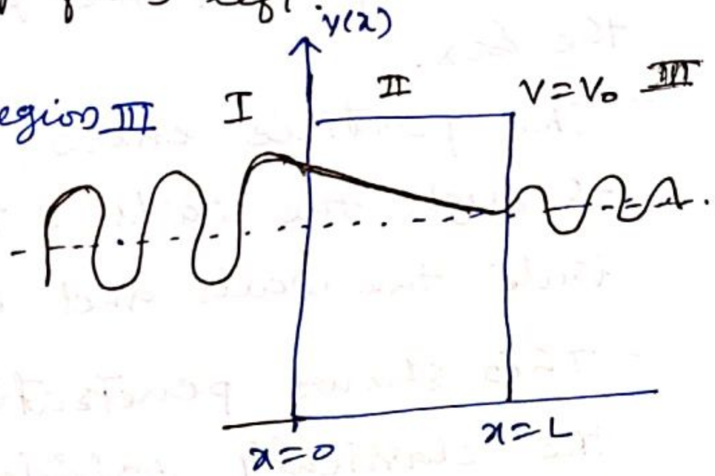


Fig: Potential barrier tunneling

- 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 $\sqrt{\frac{2(E-V_0)}{m}}$
- The particle thus transmitted into region III.
- But if $E < V_0$ the particle can not enter region II and is 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,

$$\psi_I = A e^{k'x} + B e^{-k'x} \quad \ldots (1)$$

- The first term is the incoming wave along the positive x-direction while the second term is the reflected wave moving along $-ve$ x-direction.

- In region ~~II~~ III, $V_x \hat{=} 0$ $(V_x = 0)$ for $x \geq L$ the wave function in the region is,

$$\psi_{III} = De^{-k'x} \quad \ldots \ldots (2)$$

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

$$\psi_{II} = Pe^{ikx} + Qe^{-ikx} \quad \ldots (3)$$

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

i.e.
$$\left.\begin{aligned} \psi_1 &= \psi_2 \\ \frac{\partial \psi_1}{\partial x} &= \frac{\partial \psi_2}{\partial x} \end{aligned}\right\} \text{at } x=0$$

$$\left.\begin{aligned} \psi_{II} &= \psi_{III} \\ \frac{\partial \psi_{II}}{\partial x} &= \frac{\partial \psi_{III}}{\partial x} \end{aligned}\right\} \text{at } x=L$$

- 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 incidenteing on the potential barrier with energy less than the height of the potential barrier, there is always some probability of transmission through the barrier.
- This phenomenon of crossing the barrier is called the 'Tunneling Effect'.

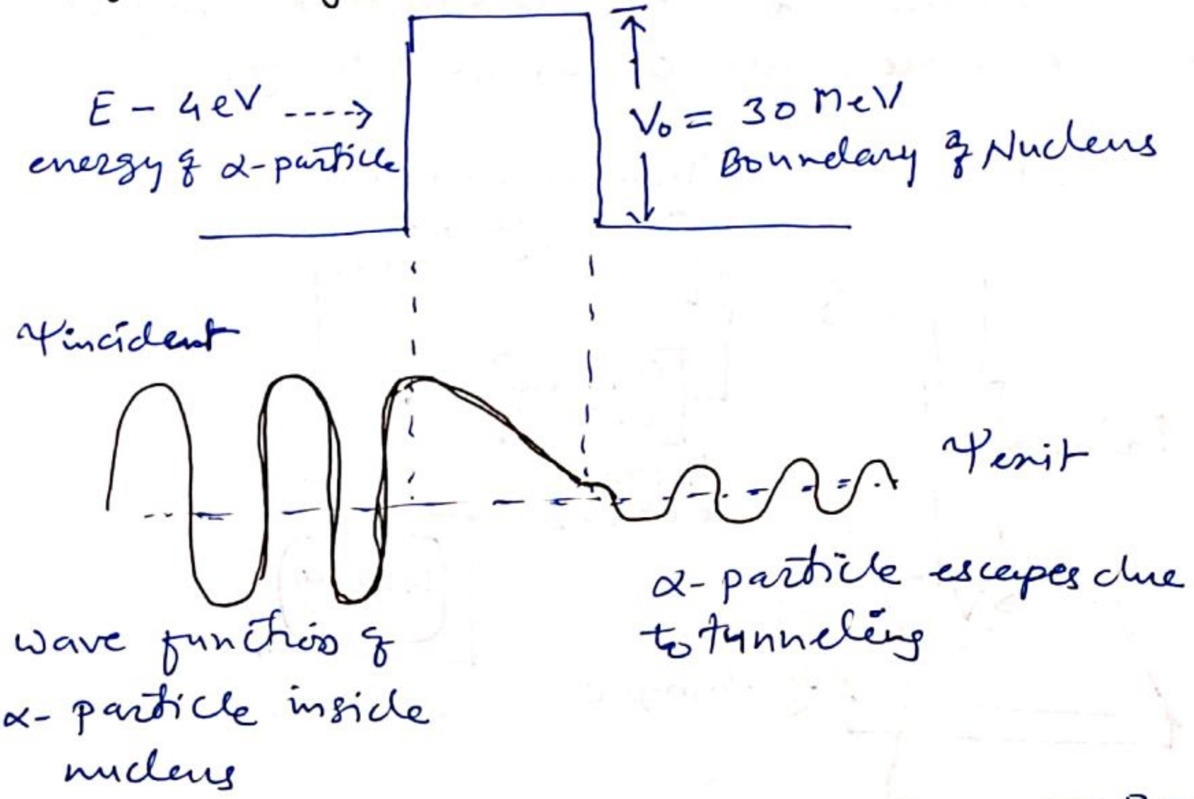
—o—o—o—o—o—o—

Applications of Tunneling

1. α- decay

1. In α- ~~day~~ decay, an unstable nucleus disintegr-ates into a lighter nucleus and ~~and~~ α- particle.
2. i.e Uranium nucleus ^{238}U undergoes α- decay and forms thorium nucleus ^{234}Th.
3. In 1928 George Gamow explained α- decay of unstable nuclei on the basis of quantum tunneling
4. The forces in the nucleus set up a potential barrier of height of the order of 30 MeV against α- particle emission.
5. According to classical mechanics, the α- particle would be trapped unless its energy exceeds 30 MeV.
6. The α- particle have energies in the range of 4 to 9 MeV only.
7. Therefore it is impossible for a α- particle to cross the barrier.
8. According to quantum mechanics, the α-particle tunnels through the potential barrier.

Fig: α-decay



Scanning Tunneling Microscope. (STM)

1. STM was invented in 1979 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 betw 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

- of the distance betn two conducting samples. The STM makes use of this sensitivity.

Working:

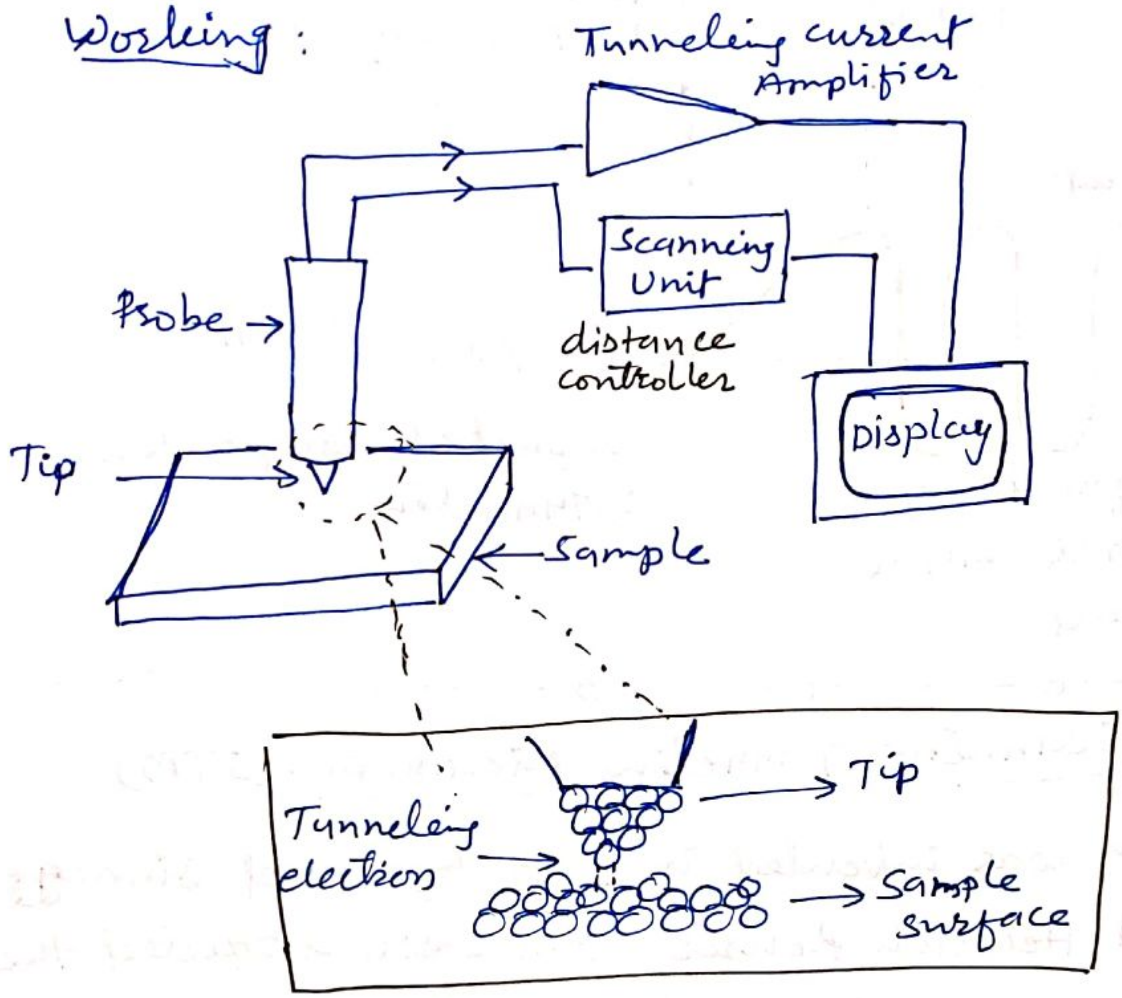


Fig. Schematic diagram of STM.

1. In scanning tunneling microscope the sample is scanned by a very finite mettallic 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 angstrons.
3. A bias voltage is applied between the sample and 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 'tunneling current' in the needle.

This feeble tunneling current is amplified and measured.

5. With the ~~help~~ help of tunneling current the feedback electronics keeps the distance betn tip and sample constant.

6. The sensitivity of the STM is so large that electronic corrugation of surface atoms and the electron distribution around them can be detected.

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

Tunnel Diode

1. Tunnel diode was invented in 1958 by Leo Esaki, who in 1973 recieved the noble prize in physics.

2. These tunel diodes have constructed by heavily doped p-n junction of only of the order of 10 nm. wide.

3. This heavy doping results in a broken bandgap where conduction band electron states on n-side are more aligned with valence band hole states on the p-side.

4. Tunnel diodes are made from Ge, GaAs & Si. they can be used as oscillators, amplifiers, frequency converters and detectors etc.

5. Under normal forward bias operation, as voltage increases, electrons at first tunnel through the very narrow p-n junction as shown in fig. below.

- This is because filled electron states in the conduction band on the n-side become aligned with empty valence band hole states on the p-side of the p-n junction.

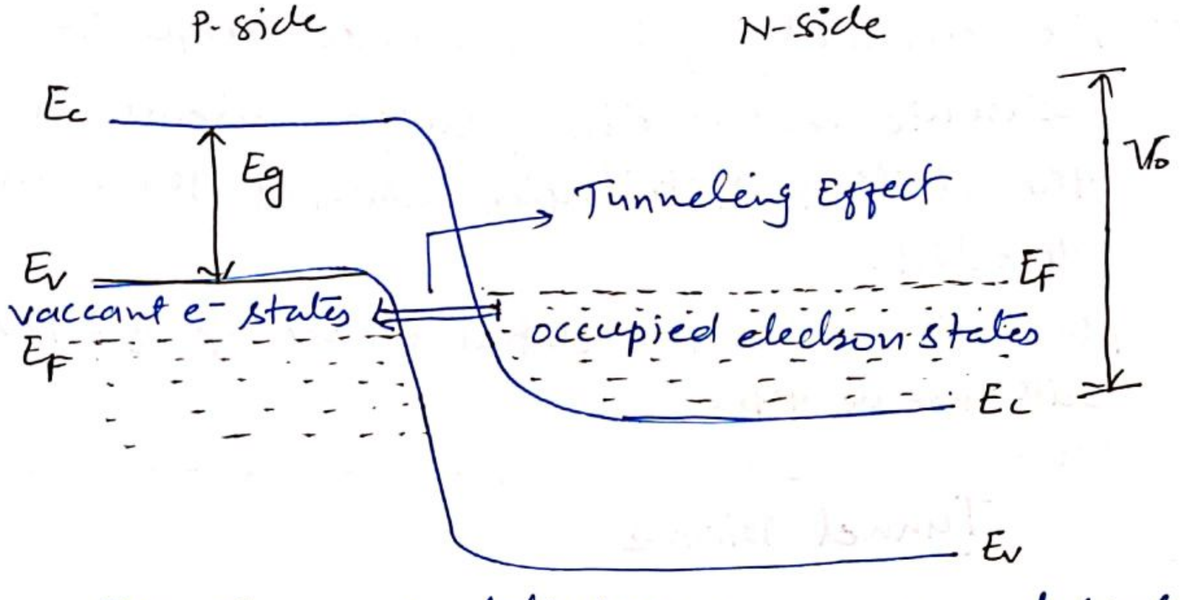


fig: Energy Band diagram ~~for~~ for tunnel diode.

6. As voltage increases further these states become more misaligned and the current drops, this is called negative resistance, because current decreases with increasing voltage.

7. As voltage increases further the diode begins to operate as a normal diode, where electrons travel by conduction across the p-n junction and no longer by tunneling through the p-n junction barrier.

8. When tunnel diodes are operated in reverse bias, can act as fast rectifiers with zero offset voltage and extreme linearity for power signals.

9. Under reverse bias filled states on the p-side become increasingly aligned with empty states on the n-side and ~~e~~ electrons now tunnel through the p-n junction barrier in reverse direction.

- This is the zener effect and can be observed in zener diodes.

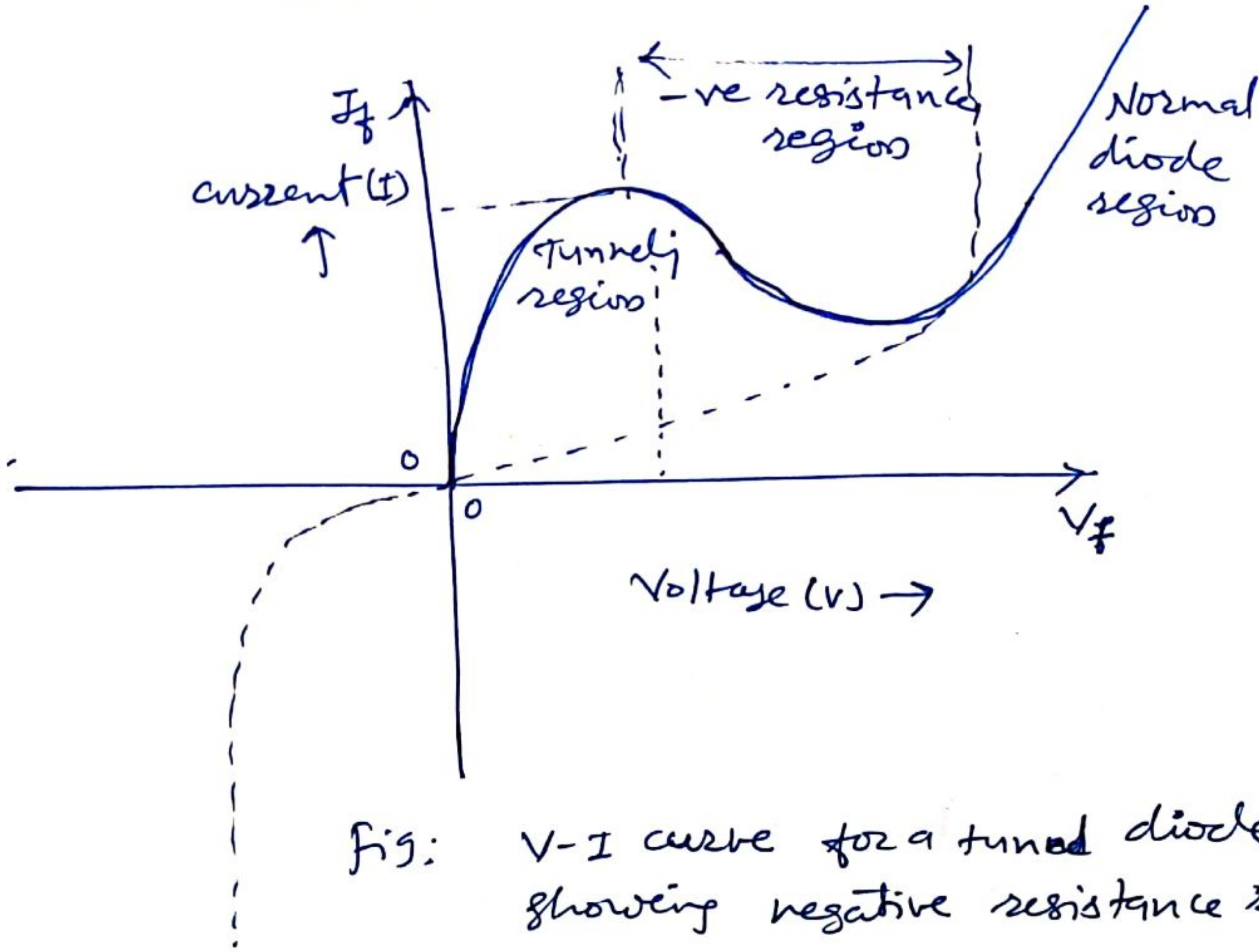


fig: V-I curve for a tunnel diode showing negative resistance region.