# Quantum Mechanics

- Branch of physics which deals with the study of behaviour of ~~par~~ matter at atomic & subatomic level.

- DE BROGLIE HYPOTHESIS :-

- 1924, Louis de Broglie extended the idea of dual nature of light to the material particles.
- As there is ~~a~~ ~~sym~~ always a symmetry in nature so if waves (light) can behave as particle; then particles should also behave like waves.
- He gave the ~~theory~~ Hypothesis :
  If light can act as a wave sometimes & as particle at other times, then particles (ex - electron) should also act as waves at times. ← De Broglie Hypothesis.
- So a moving particle will have a wave associated with it
  ⇒ just like in classical mechanics we represent ~~pos~~ a particle by its position & momentum. We can represent a moving particle in the form of wave associated with it.
  Waves associated with particles are called as 'de Broglie waves' or 'matter waves'
  And the wavelength of these matter waves / de Broglie waves ~~is~~ ($\lambda$.) associated with moving particle with velocity (v) is proportional to magnitude of momentum of particle

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

$h \rightarrow$ Planck's const $= 6.23 \times 10^{-34}$ $kg^{m}$ / sec.

* De Broglie wavelength of matter waves :-

- Consider a photon moving with speed 'c'. we can express momentum of that photon as

$$p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda} \qquad \left(\because \nu = \frac{c}{\lambda}\right)$$

$\therefore$ Wavelength & momentum p of a photon are related to each other by :

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

- He proposed this equation to be universal i.e. applicable to all photons & material particles also.

- Quntities i.e $\nu$ & $\lambda$ are related to waves but E & c are related to particle. & tied with relation:

$$\boxed{E = h\nu} \quad \& \quad \boxed{p = \frac{h}{\lambda}}$$ $\Rightarrow$ wave-particle dualism of light.

- Consider a moving particle of mass 'm' & is moving with speed v so that $p =$

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

Waves associated with moving particles are called as matter waves or de Broglie waves.

Rel$^n$ $\lambda = h/mv$ → de Broglie Equation of wavelength

$\lambda$ → de Broglie wavelength.

- It is observed that :
  - when velocity of particle is zero, $\lambda \to \infty$
    It means matter waves are detectable only for moving particles.
  - Lighter the particle, smaller the value of m & hence longer is the wavelength of matter associated with it.

- Hence, behaviour of micro-particles will be significant but ~~be~~ waves associated with macro-bodies can never be detected.
- Smaller the velocity of micro-particle, Longer is the wavelength of matter wave associted with it.

* When we consider a photon as a particle, corresponding EM wave is the de Broglie wave for photon.

~~But~~ Atomic particles ~~ar~~ also have matter waves associated with them. But it was found later that these matter waves are not real 3-D waves but "probability waves" related to probabilities of finding the particles in various places & with various properties.

* De-Broglie wavelength associated with an accelerated charged particle :-

- If a charged particle, ex - an electron is accelerated by a potential difference of 'V' volts,

$\therefore$ K.E of $e^-$ $\Rightarrow$ K.E = eV.

$$\therefore \frac{1}{2}mv^2 = eV \Rightarrow v = \sqrt{\frac{2eV}{m}}$$

Electron wavelength is given by:

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

$$\boxed{\lambda = \frac{h}{\sqrt{2eVm}}}$$

$m_e = 9.1 \times 10^{-31}$ kg
$h = 6.625 \times 10^{-34}$ J/sec
$e = 1.6 \times 10^{-19}$ C

$$\therefore \boxed{\lambda = \frac{12.27}{\sqrt{V}} \mathring{A}}$$

* De-Broglie wavelength expressed in terms of K.E:

If particle has K.E, $K.E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m}$

$$p = \sqrt{2m(K.E.)}$$

$$\therefore \boxed{\lambda = \frac{h}{\sqrt{2m(K.E.)}}}$$

* De Broglie wavelength associated with particles in thermal equilibrium :-

↳ If ø particles are in thermal equilibrium at temp T
K.E. at Thermal equilibrium at T

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

k → Boltzman const.

$$\therefore \lambda = \frac{h}{\sqrt{2m(K.E)}} = \frac{h}{\sqrt{3mkT}}$$

$$\boxed{\lambda = \frac{h}{\sqrt{3mkT}}}$$

* Concept of Group Velocity & phase Velocity :-

- We know, at microscopic levels wavelength of de Broglie wave which is associated with every material particle becomes important.
Speed with which a crest or trough of wave travel is called 'phase velocity' of the de Broglie waves. also called 'wave velocity'
For this wave ~~p~~ velocity, phase remains ~~same~~ constant.

* For a particle of mass 'm', moving withe the velocity 'v', de Broglie wavelength is

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

We know, energy, $E = h\nu = mc^2$

$$\Rightarrow \quad \nu = \frac{mc^2}{h}$$

For a wave with frequency $(\nu = mc^2/h)$ & wavelength $\lambda$. , we can write eqⁿ of motion as :

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

$\omega = 2\pi\nu$ : Angular frequency

$k = \frac{2\pi}{\lambda}$ → Propagation const of wave.

For wave with constant phase :

$\omega t - kx = \text{const.}$ ⇒

Differentiating eqⁿ :

$\omega\, dt - k\, dx = 0 \Rightarrow \omega\, dt = k\, dx$

$\Rightarrow \boxed{\frac{dx}{dt} = \frac{\omega}{k}}$ we know, $\frac{dx}{dt}$ = velocity $v$

$\therefore \boxed{v = \frac{\omega}{k}}$

Substitute $\omega$ & $k$ value →

$\therefore v = \frac{2\pi\nu}{2\pi/\lambda} = \nu\lambda.$ $\therefore \boxed{v_p = \nu\lambda}$

$\nu$ → Frequency of matter waves.

Also, $v = \frac{mc^2}{h} \cdot \frac{h}{mv}$ $\left(\because \nu = \frac{mc^2}{h} \ \& \ \lambda = \frac{h}{mv}\right)$

$$\boxed{v_p = \frac{c^2}{v}}$$

Phase velocity → always greater than c as v is always less than c

Which is an unexpected result.

This Difficulty can be overcome by ~~con~~ group velocity I.

* Group Velocity :-

- A material particle can be ~~p~~ represented by a wave packet or the group of waves & velocity of these waves is 'group velocity'

Individual waves travel inside the group with their phase velocities / wave velocities.

- A group can be obtained by interference of many waves of different frequiencies & amplitudes so that resultant has a high value of amplitude near the vicinity of particle & gets attenuated outside this region.

We can say particle is somewhere in wave packet & wave packet moves with velocity of particle carrying that particle in it.

Group of waves

Consider two waves of equal ~~ma~~ amplitude 'a' but different angular frequencies $\omega_1$ & $\omega_2$ & propagation constant $k_1$ & $k_2$

$\therefore$ $Y_1 = a \sin(\omega_1 t - k_1 x)$ &

$Y_2 = a \sin(\omega_2 t - k_2 x)$

$\therefore$ Resultant : $Y = Y_1 + Y_2 = a\left[\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)\right]$

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

$$\sin\left[\frac{(\omega_1 + \omega_2)t}{2} - \frac{(k_1 + k_2)}{2}x\right]$$

$\because \left[\sin A + \sin B = 2\sin\left(\frac{A+B}{2}\right)\cdot\cos\left(\frac{A-B}{2}\right)\right]$

$\therefore$ Resultant wave has angular frequency $(\omega_1 + \omega_2)/2$

& amplitude :-

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

$\therefore$ Amplitude of wave packet varies with $x$ & $t$ such variation in amplitude is 'modulation' of wave

* A wave of angular ~~velocity~~ ~~$\omega$~~ frequency $\omega$ & propagation const $k$, moving with velocity

$$v_p = \frac{\omega}{k} = \nu\lambda. \quad \&$$

2nd wave of Angular freq $\Delta\omega/2$ & propagation const $\Delta k/2$ moving with velocity

$$v_g = \frac{\Delta\omega}{\Delta k}.$$

$\Delta\omega$ & $\Delta k \to$ very small

$$\therefore \boxed{v_g = \frac{d\omega}{dk}.} \Rightarrow v_g = \frac{2\pi\, d\nu}{2\pi d(1/\lambda)} = -\lambda^2\frac{d\nu}{d\lambda}.$$

* Relationship between Phase Velocity & Group Velocity :-

Velocity of individual component wave of wavepacket velocity

$$v_p = \nu\lambda$$

using, $\nu = \omega/2\pi$ & $\lambda = 2\pi/k$.

$$\therefore v_p = \frac{\omega}{2\pi}\cdot\frac{2\pi}{k} = \frac{\omega}{k}. \Rightarrow \underline{\omega = k v_p.}$$

Group velocity : $v_g = \frac{d\omega}{dk} = \frac{d}{dk}(k v_p)$

$$v_g = v_p + k\frac{dv_p}{dk}$$

$k = \frac{2\pi}{\lambda}$ $\therefore dk = -\frac{2\pi}{\lambda^2}d\lambda$

$$\therefore \frac{k}{dk} = -\frac{\lambda}{d\lambda}$$

$$\therefore \boxed{v_g = v_p - \lambda\frac{dv_p}{d\lambda}.}$$ ← Rel$^n$ bet$^n$ $v_p$ & $v_g$

When entire constituent waves travel with same velocity as phase velocity $\Rightarrow$ $v_g = v_p$

$\therefore$ For non dispersive medium $\Rightarrow$ $\underline{v_g = v_p}$

Waves with different wavelength travel with different speeds in a medium.

$\therefore$ In general, group velocity is less than the phase velocity.

* Heisenberg Uncertainty Principle :-

In classical mechanics, we can decide state of a particle by ~~defining~~ specifying its position & momentum at any given time t.

A body is moving along x-direction with velocity v its position is given by $x = vt$. & momentum $p = mv$

$$\therefore \boxed{x = \frac{p}{m} t}$$

At any instant position & momentum can be measured to a very high accuracy.

But when we consider particles of small size (atomic & subatomic level) there will be restriction on precision by de Broglie wave packet.

↳ Moving microparticles are equivalent to a wave packet. A wave packet spreads over a region of space. Hence it will be difficult to locate exact position of microparticle. Even though particle will be in wavepacket it will be impossible to find the exact position of the particle.

If linear spread of wave packet is $\Delta x$, particle would be located somewhere within region $\Delta x$.

Probability of finding that particle is maximum at the centre of wave packet & falls off to zero at its ends.

Hence, there is uncertainty ($\Delta x$) in the position of particle. Because of which we can not measure momentum of particle at that instant, precisely.

⇒ Location & momentum of a microparticle can not be simultaneously determined with certainty.

If we try to determine one variable, other ~~op~~ variable will be uncertain.

∴ 1927, Heisenberg showed that the product of uncertainty $\Delta x$ in x-coordinate of a quantum particle & uncertainty $\Delta P_x$ in x-component of momentum would always be of order of Planck's constant h.

$$\therefore \quad \Delta x \cdot \Delta P_x \approx h$$

$$\Rightarrow \boxed{\Delta x \cdot \Delta P_x \geq \frac{\hbar}{2}}$$

This is known as Heisenberg's uncertainty principle for position & momentum.

It's stated as:

"It is not possible to know simultaneously & exactly both position & momentum of a microparticle."

- In classical mechanics precision of any measurement was limited only by accuracy of instruments used, Heisenberg showed that whatever may be the accuracy of instrument used, quantum mechanics limits the precision when two properties are measured at same time.

These two quantities are such that product of

these quantities has dimensions of "energy × time"
Such quantities are "Conjugate Quantities" in Q.M.
ex → Position - linear momentum, energy - time, time - frequency & angular momentum - angular displacement
↑ conjugate pairs.

∴ # Uncertainty principle asserts that it is physically impossible to know simultaneously exact position ($\Delta x = 0$) & exact momentum ($\Delta P = 0$) of a micro-particle.
∴ more precisely we know position of the particle, the less precise is our information about its momentum.
∴ momentum of a particle can not be precisely specified without our loss of knowledge of the position of particle at that time. & a particle can not be precisely localized in a particular direction without our loss of knowledge of momentum in that particular direction.
Uncertainty principle implies that we can never define the path of an atomic particle with absolute precision indicated in classical mechanics.

∴ Also, $\Delta y \cdot \Delta P_y \geq \frac{\hbar}{2}$ & $\Delta z \cdot \Delta P_z \geq \hbar/2$

* Energy - Momentum Uncertainty :-
Uncertainty relⁿ for simultaneous measurement of energy E & time t → $\boxed{\Delta E \cdot \Delta t \geq \hbar/2}$

⇒ If $\Delta E$ is maximum uncertainty in the determination of energy of particle, then minimum time interval for which particle remains in that state:

$$\Delta t = \frac{\hbar/2}{\Delta E}.$$

If particle remains in particular energy state for maximum time $\Delta t$, then minimum uncertainty in particle energy $\rightarrow$ $\Delta E = \frac{\hbar/2}{\Delta t}$.

* Why electrons can not be present in the nucleus:

- Radius of nucleus is $\sim 10^{-14}$ m.

If $e^-$ would be in nucleus, maximum uncertainty $\Delta x$ in position of $e^-$ = diameter of nucleus

$$\Delta x = 2 \times 10^{-14} \text{m}.$$

$\therefore$ Min. uncertainty in momentum:-

$$\Delta p = \frac{\hbar}{\Delta x} = \frac{1.04 \times 10^{-34} \text{ Js}}{2 \times 10^{-14} \text{ m}} = 5.2 \times 10^{-21} \text{ kg-m/s}.$$

$\therefore$ The minimum energy of $e^-$ in the nucleus is given by

$$E_{min} = P_{min} \cdot c = 5.2 \times 10^{-21} \times 3 \times 10^{8} = 1.56 \times 10^{-12} \text{ J}$$

$$= \underline{\underline{9.7 \text{ MeV}}}$$

$\therefore$ To exists within nucleus $e^-$ must have energy of about 10 MeV.

And exptly found energy for $e^-$ $\rightarrow$ $\sim 4$ MeV

$\therefore$ $e^-$ can not exists inside nucleus.

* Wave function & Probability Interpretation:-

- When we consider a particle behaving as a wave there will be a wave associated with it (de Broglie wave) & we can represent a wave by a wave function

$\therefore$ We represent that wave by a funcⁿ '$\psi$' $\rightarrow$ wave funcⁿ. & it is funcⁿ of $\underline{\underline{\text{position}}}$ & time.

- No direct physical significance as it is not an observable quantity
As we can not know exact value but a probable value in a measurement.
Probability can not be negative.
$\therefore \psi$ can not measure exact $(x, y, z)$ presence of particle. but it is certain that it is in someway an index of presence of particle at around $(x, y, z)$.

* Probability interpretation of wave fucⁿ given by Max Born :

↳ square of magnitude of wave fucⁿ $|\psi|^2$ evaluated in a particular region represents Probability of finding the particle in that region.
Probability of finding a particle in an infinitsimal Volume $dV$ $(= dx\, dy\, dz)$ is →

$$P \propto |\psi(x, y, z)|^2 \, dV.$$

$|\psi|^2 \rightarrow$ Probability density &
$\psi \rightarrow$ Probability amplitude.

- Since particle is ~~ert~~ certainly somewhere in the space, probability $= 1$ & hence integral of $|\psi|^2 dV$ over Entire space must be equal to 1.

$$\therefore \int_{-\infty}^{\infty} |\psi|^2 dV = 1$$

wave fucⁿ $\psi$ is in general a complex function.
$\therefore$ To make probability some real value, $\psi$ is multiplied by its ~~com~~ complex conjugate $\psi^*$.

$$\boxed{\therefore \int_{-\infty}^{\infty} \psi \psi^* \, dv = 1}$$

$\psi$ as such has no any physical significance but $|\psi|^2$ gives probability of finding the atomic particle in a particular region.

* Normalization condition :-

If a particle exists in a space, we are certain about finding that particle in entire space.
$\therefore$ probability $(\int |\psi(x,y,z,t)|^2)$ will be unit.

If $\psi(x,y,z,t)$ is multiplied by some constant 'C' such that $\psi_N(x,y,z,t) = C\,\psi(x,y,z,t)$

$\psi_N(x,y,z,t)$ satisfies the reln :

$$\int_{-\infty}^{\infty} |\psi_n(x,y,z,t)|^2 \, dx\,dy\,dz = |C|^2 \int_{-\infty}^{\infty} |\psi(x,y,z,t)|^2 dx\,dy\,dz$$
$$= 1.$$

then we can say $\psi_N(x,y,z,t)$ is normalized &

$C \rightarrow$ Normalization constant

$$\boxed{\int_{-\infty}^{\infty} |\psi_N(x,y,z,t)|^2 dx\,dy\,dz = |C|^2 \int_{-\infty}^{\infty} |\psi(x,y,z,t)|^2 dx\,dy\,dz = 1}$$

Normalization condition

$|\psi_N(x,y,z,t)|^2 \, dx\,dy\,dz \rightarrow$ Probability Density.

* Whenever wave functions are normalised, $|\psi|^2 dV$ equals the probability that a particle will be found in an elemental volume $dV$.

$\therefore$ probability $\boxed{P = |\psi(x,y,z)|^2 \, dV}$.

* Well behaved wave functions :

Conditions to be satisfied by $\psi$- function :-

- An acceptable wave fucn $\psi$ must be normalized & fulfill following requirements :

(I) $\psi$ function must be finite :

- wave fucn must be finite everywhere
- If $x \to \infty$ or $-\infty$, $y \to \infty$ or $-\infty$, $z \to \infty$ or $-\infty$ wave fucn should not tend to infinity
- It must remain finite for all values of $x, y, z$.
- If $\psi$ is infinite, it would imply that probability of finding particle will also be infinite. (large) which violate the uncertainty principle.

(II) $\psi$ function must be single-valued :

Any physical quantity can have only one value at a point.

$\therefore$ Fucn related to physical quantity can not have more than one value at a point,

~~is~~ If it has more than one value at a point it means that there is more than one value of probability of finding particle at that point.

(III) $\psi$ Function must be continuous :

As $\psi$ is related to a physical quantity, it can not have discontinuity at any boundary

Hence, wave fucn $\psi$, & its space derivatives $\frac{\partial \psi}{\partial x}$, $\frac{\partial \psi}{\partial y}$ & $\frac{\partial \psi}{\partial z}$ should be continuous across any boundary

- Wave fucn satisfying above conditions is called "well-behaved wave fucn"

# * SCHRÖDINGER WAVE EQUATION :-

- Schrödinger Equation :

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi} \rightarrow \text{1-D eq}^n. \quad - \text{I}$$

We want to know the wave fuc$^n$ i.e. $\psi$.
We can get that wave fuc$^n$ $\psi$ by solving schrödinger eq$^n$ :-
We have, schrödinger eq$^n$ for 1-D along $X$-axis !

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi . \quad - \text{II}$$

$\psi \Rightarrow \psi(x,t)$ $\psi$ is fuc$^n$ of $x$ & $t$.

So we can find '$\psi$' be separation of variables

$\therefore$ We assume two sol$^n$ for $\psi(x,t)$ I

$$\psi(x,t) = \psi(x)\,\phi(t) \quad - \text{III}$$

$\therefore$ For separable sol$^n$ :

By taking derivative $\rightarrow$ $\frac{\partial \psi}{\partial t} = \psi \frac{\partial \phi}{\partial t}$ ; Also, $\frac{\partial^2 \psi}{\partial x^2} = \frac{d^2 \psi}{dx^2}\phi$

Diag

$$\therefore i\hbar\, \psi . \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{d^2 \psi}{dx^2}\phi + V\psi\phi .$$

By substituting $d\psi/dt$ & $d^2\psi/dx^2$ in eq$^n$ II

Now, divide by $\psi\phi$.

$$\therefore \frac{i\hbar}{\phi}\frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{d^2 \psi}{dx^2}\frac{1}{\psi} + V .$$

LHS is fuc$^n$ of $t$ alone & RHS is fuc$^n$ of $x$ alone.

This will be true only when both sides are constant.

| | |
|---|---|
| lec | - |
| prac | - |

$\therefore$ So let constant $= E$.

$\therefore \quad i\hbar \dfrac{1}{\phi} \dfrac{\partial \phi}{\partial t} = E$ &

$$\boxed{-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{\partial^2 \psi}{\partial x^2} + V = E}$$

$\hookrightarrow$ $$\boxed{-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi = E\psi}$$

Schrödinger's time independent eq$^n$.

* For time-Dependent schrödinger's eq$^n$:

$$i\hbar \frac{1}{\phi} \frac{d\phi}{dt} = E \Rightarrow \frac{d\phi}{dt} = -\frac{iE}{\hbar}\phi$$

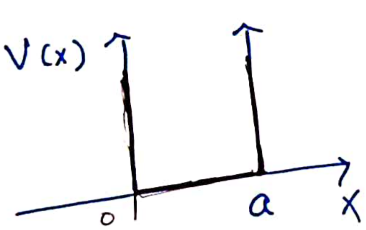
$\therefore$ Sol$^n$ $\rightarrow$ $\boxed{\phi = c \cdot \exp\left(-i\frac{E}{\hbar}t\right)}$

$c \rightarrow$ integration constant.

* We can use time independent equation for differet systems. If we have a particle with energy E & if there is potential of V. then we can find solution for schrödinger's eq$^n$ for differnt E & V.

* Application of time independent schrödinger's equation :-

- Particle enclosed in infinitely deep potential well (particle in rigid box) :-




Infinite deep potential well:

Value of potential (V) is infinite at & beyond two values of x at $x=0$ & $x=a$.

Value of potenitial (V) in that well i.e. between $0 \le x \le a$, potential is zero.

$$\therefore \quad V = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

We have a particle with energy 'E' & it is in $\infty$ deep potential well.

$\therefore$ Inside the well, $V = 0$ & $\rightarrow 0 \leq x \leq a$

outside the well, $V = \infty$ $\rightarrow$ $x > a$

$\therefore$ We can write schrödinger wave eq$^n$ inside the well ($0 \leq x \leq a$) as:

$$\therefore \quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad (\because V = 0 \text{ inside})$$

$$\therefore \quad \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}E\psi = \boxed{\frac{d^2\psi}{dx^2} = -k^2\psi}.$$

where, $k = \sqrt{\dfrac{2mE}{\hbar^2}} = \dfrac{\sqrt{2mE}}{\hbar}$.

General sol$^n$ for such eq$^u$ations :-

$$\psi(x) = A\sin kx + B\cos kx.$$

A & B $\rightarrow$ Arbitrary constants. ~~Ex~~ typically fixed by boundary cond$^n$ of the problem.

By applying boundary cond$^n$ $\rightarrow$

$$\psi(0) = \psi(a) = 0 \quad \text{(continuity)}$$

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

$$\therefore B = 0 \Rightarrow \boxed{\psi(x) = A\sin kx}$$

2$^{nd}$ cond$^n$ $\psi(a) = 0 \Rightarrow \psi(a) = A\sin ka$.

$\Rightarrow A\sin(ka) = 0 \Rightarrow$ either A or $\sin ka \Rightarrow 0$

As $\psi$ - normalized wave fuc$^n$ $\therefore A \neq 0$

$\therefore$ $\sin ka = 0 \Rightarrow ka = 0, \pm\pi, \pm 2\pi, \cdots$

$\therefore$ Distinct $sol^n$ :

$$\boxed{k_n = \frac{n\pi}{a}} \quad \text{with } n = 1, 2, 3 \ldots$$

$\therefore$ Possible values of $E \rightarrow$

$$k = \frac{\sqrt{2mE}}{\hbar} \Rightarrow \frac{k^2\hbar^2}{2m} = E.$$

$$\therefore \boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2a^2 m}.}$$

$\therefore$ Quantum particle in $\infty$ square well can not have just any value of energy but it has to be one of these special allowed values.

$\therefore$ For Normalized $\psi$

$\psi = A \sin kx$, we can find const $A$

Normalization $cond^n$

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \Rightarrow \int_0^a |A|^2 \sin^2 kx \, dx = 1$$

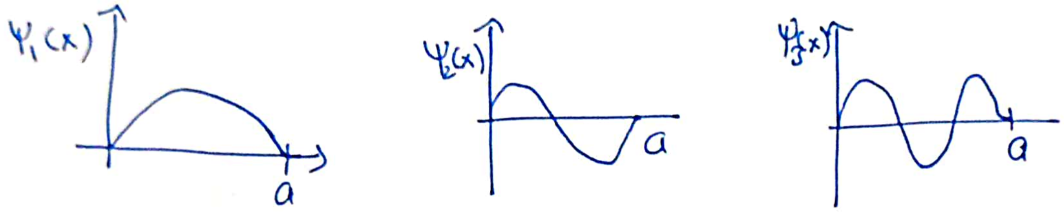
$$\Rightarrow |A|^2 = \frac{1}{\int_0^a \sin^2 kx \, dx} \quad \left[\sin^2 kx = \frac{1}{2}(1 - \cos 2kx)\right]$$

$$\therefore |A|^2 = \frac{1}{\frac{1}{2}\int_0^a 1 - \cos 2kx} = \frac{1}{\frac{a}{2} - a\left[\frac{\sin 2kx}{2}\right]_0^a}$$

$$= \frac{1}{a/2} \Rightarrow |A|^2 = \frac{2}{a} \Rightarrow \boxed{A = \sqrt{\frac{2}{a}}}$$

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

Time-independent Schrödinger $eq^n$ has given an infinte set of $sol^n$ (One for each +ve integer $n$)



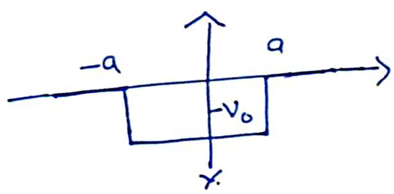

for $n=1$ for $n=2$ for $n=3$.

→ all these look like a standing waves on string of length $a$ &

$\psi_1$ → carries lowest energy is called ground state.

& others whose energy is propotional to $n^2$ → Excited states.

② Particle in Finite potential well (Particle in Non-Rigid Box)




$$V(x) = \begin{cases} -V_0 & \text{for } -a < x < a \\ 0 & \text{for } |x| > a. \end{cases}$$

$V_0 \rightarrow$ +ve const.

This potential admits both states :

for $(E<0)$ bound state & $(E>0)$ scattering state.

∴ Schrödingers eqⁿ :

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \text{or} \quad \frac{d^2\psi}{dx^2} = k^2\psi$$

$$k = \frac{\sqrt{-2mE}}{\hbar}. \quad \text{is real \& +ve.}$$

∴ solⁿ → $\boxed{\psi(x) = Be^{kx}}$ for $x < -a$.

In region, $-a < x < a$, $V(x) = -V_0$

$$\therefore -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \Rightarrow \frac{d^2\psi}{dx^2} = -l^2\psi.$$

$$l = \frac{\sqrt{2m(E+V_0)}}{\hbar}.$$

$\therefore$ sol$^n$ $\rightarrow$

$$\psi(x) = \begin{cases} Fe^{-kx} & ; x > a \\ D\cos(lx) & ; 0 < x < a \\ \psi(-x) & ; x < 0 . \end{cases}$$

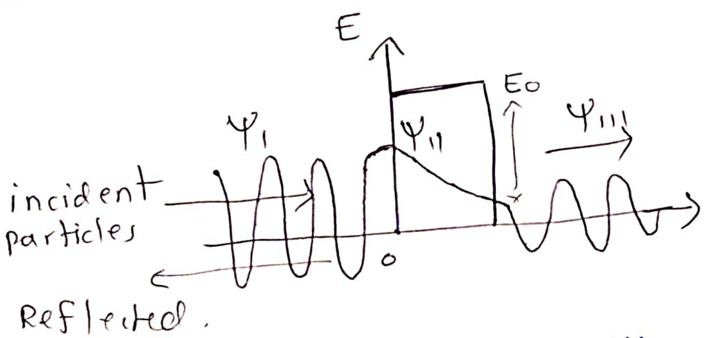
$\therefore$ Energy : $\boxed{E_n + V_0 = \dfrac{n^2\pi^2\hbar^2}{2m(2a)^2}}$

* According to classical idea, particle striking a hard ball has no chance of leaking through it. But behaviour of a quantum particle is different because of wave nature associated with it.

When EM strikes at interface of two media it is partially reflected & partly transmitted through interface of two media.

In the same way de Broglie wave also has a possibility of getting partially reflected from the boundary of potential well & partially penetrating through barrier.

Penetration of a barrier by a quantum particle is called <u>tunneling</u>




Probability that particle will penetrate the potential barrier having length L. Such penetration is tunnel effect. Probability that particle gets through barrier is called - transmission coefficient.

Transmission Coefficient (T)

$$T = \frac{\text{Probability density of the transmitted wave}}{\text{Probability density of incident wave}}.$$

* Applications of Tunnelling :-

① $\alpha$ - Decay :-

- In $\alpha$-decay, an unstable nucleus (radioactive nucleus) disintegrates into lighter nucleus & an $\alpha$-particle.

  Ex Uranium nucleus

$$^{238}U \xrightarrow{\alpha\text{ - Decay}} {}^{234}Th + \alpha .$$

- In 1928, George ~~Gamma~~ Gamow explained $\alpha$-decay of an unstable nuclei on the basis of quantum tunneling.

  ~~Forces~~ Because of forces inside the nucleus, nucleus set up a potential barrier of about 30MeV. That means if a particle wants to come out of nucleus it has to overcome that barrier / it should have energy around that barrier ht (~30MeV)

- $\alpha$- particles have energy of 4 to 9 meV only.

∴ Classically it is impossible for $\alpha$-particle to overcome that barrier.

But experimently $\alpha$ - particles are observed to be emitted from nucleus & it is because of the quantum tunnelling.

## ② Tunnel Diode :-

- Tunnel diode is a semiconductor diode.
- When p & n type semiconductors are combined in pn diode a p-n junction is formed. at this pn junction there is recombination of holes & electrons because of which a neutral deplation layer is formed.
- ~~This d~~ This deplation layer acts as a potential barrier if a $e^-$ or hole wants to go to other region it has to overcome this potential barrier.
- Electrons cross this potential barrier because of quantum tunnelling.
- By ~~appliping~~ varying applied voltage, we can control height of this barrier.

## ③ Scanning tunnelling ~~electrons~~ electron microscope (STM)

- Instrument invented by Gerd Binnig & Heinrich Rohrer for which they have got Noble prize in Physics
STM uses electron tunneling to produce images of surface down to the scale of individual atoms.
- If two conducting samples are brought in close proximity, with a small but finite distance between them, electrons from one sample flow into the other if distance is of order of the spread of electronic wave into space. Electrons tunnel through the barrier into adjacent sample.
For electrons, barrier width which may be overcome via a tunneling process is of order of nm i.e. of order of several atomic spacings.
Probability of an electron to get through tunneling barrier decreases exponentially with barrier width i.e. tunneling current is extremely sensitive measure of distance betn two conducting samples.

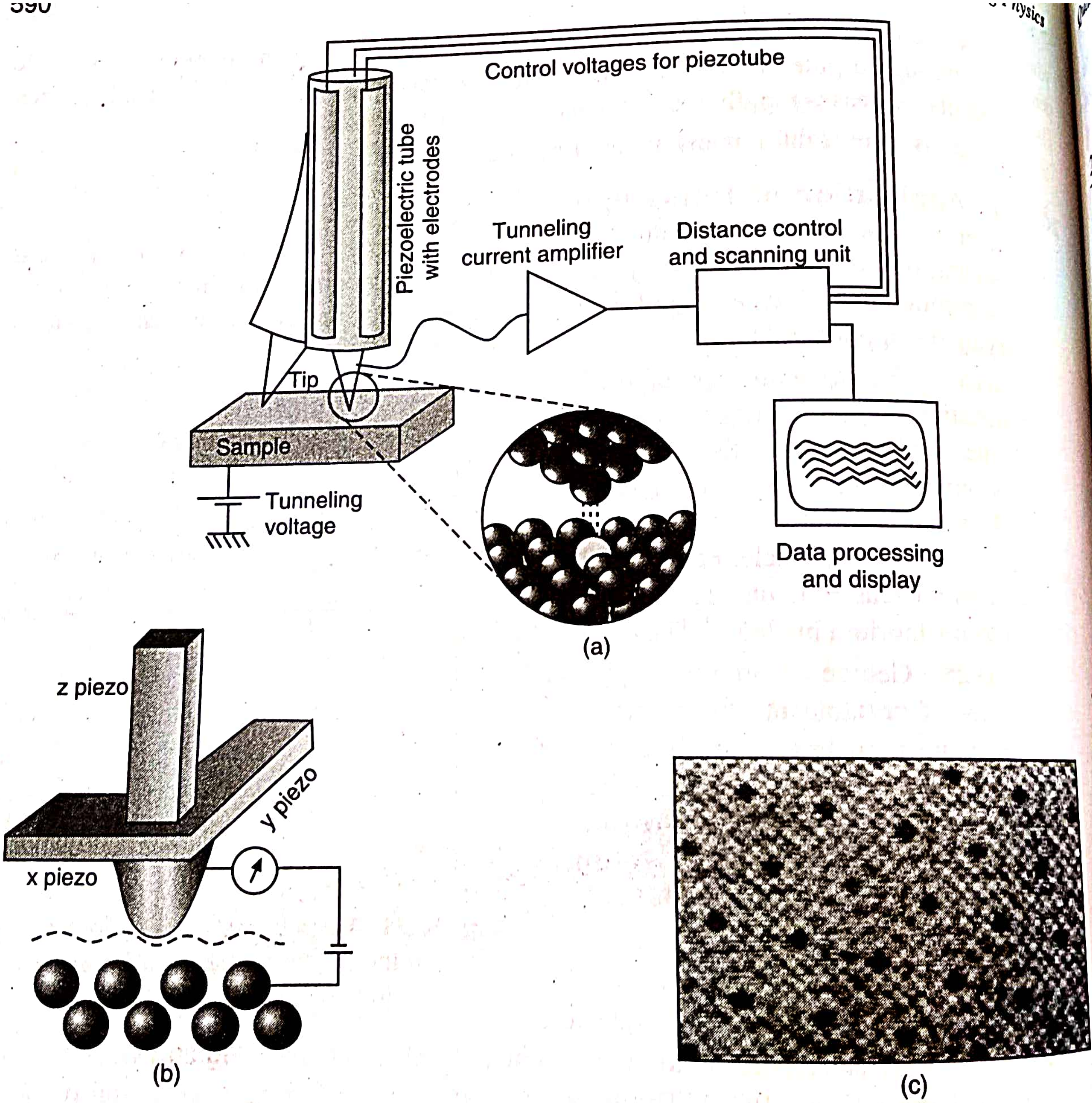



**Fig. 20.22:** (a) The schematic diagram of STM (b) The tunneling tip is scanned over the specimen, producing an image of the tunneling current (c) An image of a silicon crystal surface produced by a STM.

In STM, sample is scanned by a very fine metallic tip. Tip is mechanically connected to a scanner. The sharp metal needle is brought close to the surface to be imaged.
Distance betn sample surface & metal tip is of order of few angstroms.
A bias voltage is applied betn tip & sample.
Electron from metal tip tunneled constitutes the 'tunneling current'. in the needle.
Tunneling current then amplified & measured.

* Quantum Computing :-

- Use of quantum phenomena like superposition & entanglement to perform computation.
  Computers that perform quantum computations are known as quantum computers.
- In classical computers information is stored in the bits (either 1 or 0.) We can not get information of states which are in betn 1 & 0.
- In quantum computers information is stored in 0&1 & in addition to that, states are there which are in betn these 0 & 1. → 'qubits'
  Information is stored in the form of 'qubit'.
- Quantum computers can perform calculations within very short time as compared to classical computers. & also can store large/huge amount of data.