QUANTUM MECHANICS

Quantum mechanics deals with the **systematic investigation (study) of the mechanical behavior of microparticles like molecules, atoms, electrons, nucleus, nucleons etc**. It also explains the mechanics of macroparticles as well.

Classical Mechanics	Quantum Mechanics
Deals with the mechanics of macroparticles like objects in our daily life	Deals with the mechanics of microparticles like molecules, atoms, electrons, nucleus, nucleons etc. It also explains the mechanics of macroparticles as well.
Classical Mechanics treated particles and radiations (waves) as distinct entities, i.e. particles as particles and waves as waves alone.	According to Quantum Mechanics, radiations and material particles have dual nature. Q.M considers the wave nature of particle and particle nature of radiations as well.
The foundations of Classical Mechanics are Newtonian mechanics, thermodynamics, Maxwell's Electromagnetic theory and statistical physics.	The foundations of Quantum Mechanics are Schrodinger's wave mechanics (based on de-Broglie hypothesis of wave-particle duality) and Heisenberg's Matrix mechanics.

<u>De-Broglie hypothesis and matter waves</u>:

De-Broglie hypothesis says that **every moving material particle exhibit wave like properties under suitable conditions**, i.e. just like radiations, particles also have a dual nature. They behave like particles and waves. The **waves associated with moving material particles are called d-Broglie waves or matter waves**.

<u>Expression for de-Broglie wavelength</u>:

$$mc^2 = h\nu$$
$$mc \times c = h\nu$$
$$pc = h\nu$$
$$p = \frac{h\nu}{c}$$

Consider a photon of light of frequency ν, the momentum of the photon $p = \frac{h\nu}{c}$

Here $c = \nu\lambda$ or $p = \frac{h\nu}{\nu\lambda} = \frac{h}{\lambda}$. Therefore, the wavelength of the photon $\lambda = \frac{h}{p}$ ----(1)

De-Broglie suggested that the equation $\lambda = \frac{h}{p}$ is completely a general one that applies to photons as well as to material particles.

Thus de-Broglie wavelength of a moving material particle $\boxed{\lambda = \frac{h}{p} = \frac{h}{mv}}$ ---(2)

Where m is the mass of the particle and v is the velocity.

Notes: If E is the kinetic energy of the particle, $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ or $p = \sqrt{2mE}$, then $\boxed{\lambda = \frac{h}{\sqrt{2mE}}}$

* <u>de-Broglie wavelength of electrons</u>:

Consider an electron of mass 'm' and charge 'e' is accelerated through a potential of 'V' volts. If 'v' is the velocity acquired by the electron. Then, $\frac{1}{2}mv^2 = \frac{p^2}{2m} = eV$ or $p = \sqrt{2meV}$

$$\therefore \quad \lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}$$

Substituting the values of m, e and h, we get $\boxed{\lambda = \sqrt{\frac{150}{V}}\ A^0 = \frac{12.247}{\sqrt{V}} A^0}$.

<u>Heisenberg's Uncertainty Principle</u>:

According to Heisenberg's uncertainty principle **it is impossible to measure both the exact position and momentum of an object simultaneously**.

The product of the uncertainty in the measurement of position of the particle at a certain instant and the uncertainty in the measurement of momentum of the particle at the same instant is of the order of Plank's constant 'h'.

If Δx is the uncertainty (error) in the measurement of the position of the particle along the X-direction and Δp_x is the uncertainty in the measurement of its momentum, then

$$\Delta x.\Delta p_x \geq \frac{\hbar}{2} \quad \text{or} \quad \boxed{\Delta x.\Delta p_x \approx \hbar} \quad \text{(in many practical calculations)}$$

If Δx is small, Δp_x becomes large and vice versa. Similar relations can be written for other pairs of canonical variables.

$$\Delta y.\Delta p_y \geq \frac{\hbar}{2} \quad , \quad \Delta z.\Delta p_z \geq \frac{\hbar}{2} \quad , \quad \Delta\theta.\Delta L_z \geq \frac{\hbar}{2}$$

Here θ is the angular displacement and L_z is the corresponding angular momentum.

$\Delta t.\Delta E \geq \frac{\hbar}{2}$, here t is the time and E is the energy of the particle.

<u>Applications of Uncertainty Principle</u>:

1) <u>Nonexistence of electrons inside the nucleus</u>.

From many experiments it is found that the nuclear diameter is of the order of 10^{-15} m. If an electron exists in the nucleus, the maximum uncertainty in the position of the electron will be of the order of the diameter. i.e $\Delta x = 10^{-15}$ m.

So the minimum uncertainty in the momentum $\Delta p = \frac{\hbar}{\Delta x} = \frac{6.626\times10^{-34}}{2\times3.14\times10^{-15}} = 1.055\times10^{-19}\ \text{kg m/s}$.

Then, the minimum momentum of the electron 'p' must be of the order of 1.055×10^{-19} kg m/s.

The energy of the electron (using relativistic equation)

$$E = pc = 1.055\times10^{-19}\times3\times10^{8}\,\text{J} = \frac{1.055\times10^{-19}\times3\times10^{8}}{1.602\times10^{-19}}\,\text{eV} = 198\,\text{MeV}.$$

For an electron to exist in the nucleus, it should have energy of this order. But experiments show that the energy of $\beta-$particles emitted from the nucleus does not exceed 4MeV. Hence, we conclude that electron cannot exist inside the nucleus.

2) <u>Uncertainty in the frequency of light emitted by an atom (natural broadening of spectral lines)</u>:

An atom/electron remains in the excited state for about 10^{-8} s. i.e, the maximum uncertainty in the time (Δt) can be taken as 10^{-8} s. The corresponding minimum uncertainty in energy is $\Delta E = \frac{\hbar}{\Delta t} = \frac{\hbar}{10^{-8}}$.

But we know that $E = h\nu$, then

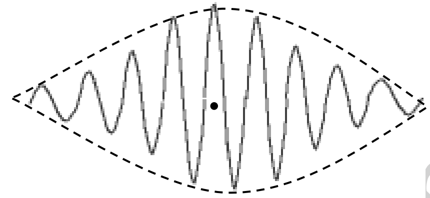
$$\Delta E = h\,\Delta\nu \ \text{ or } \ \Delta\nu = \frac{\Delta E}{h} = \frac{\hbar}{10^{-8}\times h} = \frac{h}{2\pi\times10^{-8}\times h} = 1.67\times10^{7}\,\text{Hz} = 16.7\text{MHz}.$$

This is the minimum uncertainty in frequency measurement, or this is the irreducible limit to the accuracy with which we can determine the frequency of radiation emitted by an atom.

<u>Wavepacket</u>:

According to de-Broglie hypothesis a wave is associated with a moving particle. Actually it is the resultant (envelope) of a number of waves superposed. Such **a superposed wave which is used to represent the**

wave nature of a material particle and confined (restricted) **to a small region of space in the vicinity** (neighborhood) **of the particle is called a wave packet**.
Wave packet moves with the velocity of the particle.
An ideal wave packet can be represented as shown in the figure. Here the wave has large amplitude where the particle is more expected and small amplitude where the particle is less expected.



Wave function:

The variable quantity (mathematical function) which characterizes a de-Broglie wave is known as wave function and is denoted by the symbol ψ . It is a function of both position co-ordinates and time.

i.e. $\psi = \psi(x, y, z, t)$

In general it is a complex function. Wave function itself has no physical interpretation (significance).
Characteristics of a wave function:

1) Wave function relates particle and wave nature of matter statistically.
2) Wave function is a complex quantity and cannot be measured. Hence it has no physical significance (meaning).
3) Wave function ψ and its derivatives such as $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}$ and $\frac{\partial\psi}{\partial z}$ are well behaved, i.e. single valued and continuous everywhere.
4) The probability density (probability of finding a particle in unit volume) is given by square of its magnitude. $P_d = |\psi|^2 = \psi\,\psi^*$, where ψ^* is the complex conjugate of ψ .
5) The probability of finding a particle in an elementary volume 'dxdydz' is given by $P = |\psi|^2\,dx\,dy\,dz$
6) A wave function can be normalized. i.e. if a particle is certainly to be found somewhere in a given volume, then $P = \iiint_V |\psi|^2\,dx\,dy\,dz = 1$

A wave function satisfying the above condition is called a normalized wave function.

Schrodinger time dependent wave equation:

Schrodinger wave equation is the most fundamental equation in quantum mechanics. It describes the wave nature of a particle in mathematical form. It is derived from the plane wave equation by combining with Max Plank's equation for quantum of energy and de-Broglie's equation for wavelength.
The differential equation for a de-Broglie wave propagating along the X-direction may be written as

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} ---(1)$$, here we assumed $\psi = \psi(x, t)$.

The general solution of the equation can be written as $\boxed{\psi = A\,e^{i(kx-\omega t)}} ---(2)$

where k is the wave vector $(k = \frac{2\pi}{\lambda})$ and ω is the angular frequency $(\omega = 2\pi\nu)$.

The energy of a photon having frequency ν is given by, $E = h\nu = \frac{h\omega}{2\pi} = \hbar\omega ---(a)$, where $\frac{h}{2\pi} = \hbar$

The expression for de-Broglie wavelength, $\lambda = \frac{h}{p}$, then $p = \frac{h}{\lambda} = \frac{h}{2\pi/k} = \frac{hk}{2\pi} = \hbar k ---(b)$

Using the expressions (a) and (b) in eqn (2) $\psi = A\,e^{i\left(\frac{p}{\hbar}x - \frac{E}{\hbar}t\right)}$ or $\boxed{\psi = A\,e^{\frac{i}{\hbar}(px - Et)}} ---(3)$

Differentiating eqn(3) partially with respect to x twice

$$\frac{\partial\psi}{\partial x}=\frac{\partial}{\partial x}Ae^{\frac{i}{\hbar}(px-Et)}=Ae^{\frac{i}{\hbar}(px-Et)}\cdot\frac{i}{\hbar}p=\frac{i}{\hbar}p\psi \text{ and } p\psi=\frac{\hbar}{i}\frac{\partial\psi}{\partial x} \text{ or } \boxed{p\psi=-i\hbar\frac{\partial\psi}{\partial x}}$$

$$\frac{\partial^2\psi}{\partial x^2}=\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\right)=\frac{\partial}{\partial x}\left(\frac{i}{\hbar}p\psi\right)=\frac{i}{\hbar}p\cdot\frac{\partial\psi}{\partial x}=\frac{i}{\hbar}p\cdot\frac{i}{\hbar}p\psi=-\frac{p^2}{\hbar^2}\psi$$

Or $\boxed{p^2\psi=-\hbar^2\frac{\partial^2\psi}{\partial x^2}}$ ---(4)

Differentiating eqn(3) partially with respect to t

$$\frac{\partial\psi}{\partial t}=\frac{\partial}{\partial t}Ae^{\frac{i}{\hbar}(px-Et)}=Ae^{\frac{i}{\hbar}(px-Et)}\cdot\left(\frac{-iE}{\hbar}\right)=-\frac{i}{\hbar}E\psi \text{ and } E\psi=-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} \text{ or } \boxed{E\psi=i\hbar\frac{\partial\psi}{\partial t}} \text{---(5)}$$

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

i.e. $E=\frac{p^2}{2m}+V$. Here also we are assuming $V=V(x,t)$

Multiplying by ψ we get, $E\psi=\frac{p^2\psi}{2m}+V\psi$ or $\boxed{i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi}$ ---(6)

This is the one- dimensional time dependent Schrodinger wave equation.

In three dimension, i.e if $\psi=\psi(x,y,z,t)=\psi(r,t)$ and $V=V(x,y,z,t)=V(r,t)$

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+V\psi \text{ or}$$

$\boxed{i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi}$,where ∇^2 is the Laplacian operator $\nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$

Or $\boxed{i\hbar\frac{\partial\psi}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+V\right]\psi}$ ---(7)

This is called **time-dependent Schrodinger wave equation.**

Note: for a free particle $V=0$, or Schrodinger equation becomes $\boxed{i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi}$ ---(8)

<u>Time independent Schrodinger wave equation</u> or **<u>steady state form of Schrodinger's equation</u>**.

In time dependent Schrodinger wave equation, the potential energy of a moving particle is a function of both position and time. In a number of cases, potential energy V of a particle does not depend on time explicitly; it varies with the position of the particle only and the field is said to be stationary $V=V(r)$. The wave function $\psi(r,t)$ in such cases can be expressed as a product of two functions $\phi(r)$ and $f(t)$. Here $\phi(r)$ is a function of position only and $f(t)$ is a function of time only. Thus $\psi(r,t)=\phi(r)\cdot f(t)$. Substituting this in the Schrodinger wave equation,

$$i\hbar\frac{\partial\psi(r,t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+V\right]\psi(r,t) \text{---(1)}$$

$$\phi(r)\ i\hbar\frac{\partial f(t)}{\partial t}=f(t)\left[-\frac{\hbar^2}{2m}\nabla^2+V\right]\phi(r)$$

Dividing both sides by $\phi(r).f(t)$ we get

$$\frac{1}{f(t)}i\hbar\frac{\partial f(t)}{\partial t}=\frac{1}{\phi(r)}\left[-\frac{\hbar^2}{2m}\nabla^2+V\right]\phi(r) \text{---(2)}$$

The left side of this equation is a function of 't' only, while the right side is a function of 'r' only. This is possible only if both sides are equal to a constant, and this constant is equal to the total energy E.

Thus $\frac{i\hbar}{f(t)}\frac{\partial f(t)}{\partial t} = E ---(3)$ and

$$\frac{1}{\phi(r)}\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\phi(r) = E \quad \text{or}$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\phi(r) = E\phi(r) \quad \text{or} \quad \boxed{\frac{\hbar^2}{2m}\nabla^2\phi(r) + (E - V)\phi(r) = 0} ---(4)$$

This is the time- independent Schrodinger wave equation.

This is also written as $\boxed{\nabla^2\phi(r) + \frac{2m}{\hbar^2}(E - V)\phi(r) = 0} ---(5)$

Operators in quantum mechanics:

In mathematics, an operator is a rule which transforms one function into another.

Ex: Differential operator (d/dx)

$$\frac{d}{dx}f(x) = f'(x), \quad \frac{d}{dx}x^2 = 2x$$

Or in general if the operator $\hat{A}$ transforms function f(x) into the function g(x), then we can write

$$g(x) = \hat{A}f(x)$$

In Quantum mechanics, each dynamic variable is represented as a linear operator which acts on a wave function to give a new wave function.

Momentum operator:

In one dimension, $\psi = Ae^{i(kx-\omega t)} = Ae^{\frac{i}{\hbar}(px-Et)}$

$$\frac{\partial\psi}{\partial x} = \frac{\partial}{\partial x}Ae^{\frac{i}{\hbar}(px-Et)} = Ae^{\frac{i}{\hbar}(px-Et)}\cdot\frac{i}{\hbar}p = \frac{i}{\hbar}p\psi \quad \text{and}$$

$p\psi = \frac{\hbar}{i}\frac{\partial\psi}{\partial x}$ or $p\psi = -i\hbar\frac{\partial\psi}{\partial x}$. Then momentum operator in one dimension, $\boxed{\hat{p}_x = -i\hbar\frac{\partial}{\partial x}}$

In three dimension $\boxed{\hat{p} = -i\hbar\nabla}$

Energy operator:

$$\psi = Ae^{i(kx-\omega t)} = Ae^{\frac{i}{\hbar}(px-Et)}$$

$$\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial t}Ae^{\frac{i}{\hbar}(px-Et)} = Ae^{\frac{i}{\hbar}(px-Et)}\cdot\left(\frac{-iE}{\hbar}\right) = -\frac{i}{\hbar}E\psi \quad \text{and} \quad E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t} \quad \text{or} \quad E\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Then energy operator, $\boxed{\hat{E} = i\hbar\frac{\partial}{\partial t}}$

Hamiltonian operator:

In advanced classical mechanics total energy operator is called Hamiltonian operator.

Schrodinger time independent wave equation is written as

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi(r) = E\psi(r) \quad \text{or} \quad \hat{H}\psi(r) = E\psi(r), \text{ where } \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$$

Dynamical variables	Operators
Position co-ordinates x, y, z	Position operators $\hat{x} = x,\ \hat{y} = y,\ \hat{z} = z$
Time t	Time operator $\hat{t} = t$
Momentum co-ordinates $p_x\ ,\ p_y,\ p_z$	Momentum operators $\hat{p}_x = -i\hbar\frac{\partial}{\partial x},\ \hat{p}_y = -i\hbar\frac{\partial}{\partial y},\ \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$
Momentum p	Momentum operator in three dimension $\hat{p} = -i\hbar\nabla$
Energy E	Energy operator $\hat{E} = i\hbar\frac{\partial}{\partial t}$
Kinetic energy, $K.E = \frac{p^2}{2m}$	Kinetic energy operator $\hat{K.E} = -\frac{\hbar^2}{2m}\nabla^2$
Potential energy V	Potential energy operator $\hat{V} = V$

<u>Eigen values and Eigen functions of operators</u>:

If the effect on an operator on a wave function can be written in the form

$\hat{A}\psi = \lambda\psi$, where λ is a constant. Eg: $\frac{d}{dx}e^{3x} = 3e^{3x}$

Then, the equation is called eigen value equation. Here ψ is the eigen function of operator $\hat{A}$ and λ is the eigen value of the operator.

All values of λ which are giving non-trivial solutions for the equation $\hat{A}\psi = \lambda\psi$ is called **eigen values**. [Non trivial solution – non-zero solutions. Ex: For the equation $x + 2y = 0$; trivial solution is (0,0) and non trivial solutions are (2, –1), (4, –2), etc.]

Consider the time independent Schrodinger equation

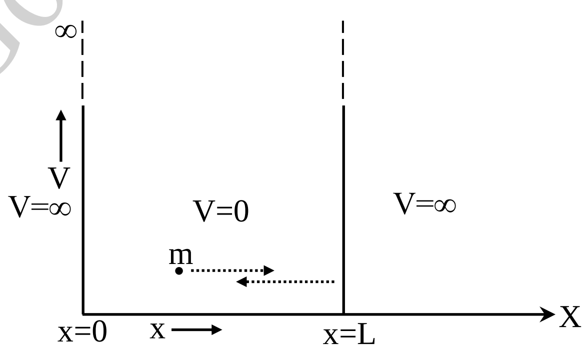
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi = E\psi\ ,\quad \text{here}\quad \psi = \psi(r)$$

This can be written as $\hat{H}\psi = E\psi$ where $\hat{H}$ is the Hamiltonian operator. This equation is an eigen value equation. This will have non-trivial solutions only for specific values of E and those values of E are called energy eigen values.

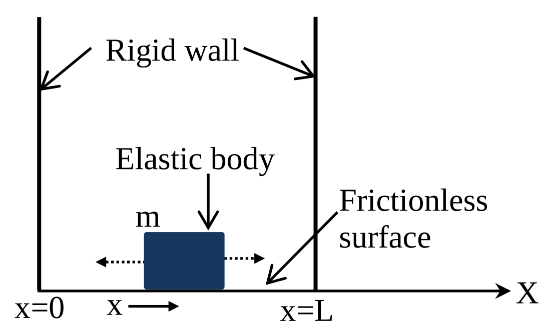
APPLICATIONS OF QUANTUM MECHANICS:

1) **<u>Particle in a One dimensional infinite square well potential</u> (particle in a one dimensional box):**

Consider a particle of mass 'm' confined in a potential well of infinite depth and finite width L, and is restricted to move in the X-direction. In order to ensure that the particle remains in the box, we shall assume that $V = 0$ everywhere at any time within the well and $V = \infty$ outside the well. Hence in this case the potential is independent of time.



Classical system



$$V(x)=\begin{cases}0 & 0\le x\le L\\ \infty & \text{otherwise}\end{cases}$$

Thus the particle is completely free in the region $0 \le x \le L$.
The time independent Schrodinger equation in one dimension is

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

Since $V=0$, $\frac{\partial^2\psi}{\partial x^2}+\frac{2mE}{\hbar^2}\psi=0$ or $\frac{\partial^2\psi}{\partial x^2}+k^2\psi \quad ---(2)$ where $k^2=\frac{2mE}{\hbar^2}$

The solution of the above equation will be of the form $\psi = A\sin kx + B\cos kx \quad ---(3)$
Since the particle is inside a square well potential of infinite depth, it is impossible to find the particle outside. i.e, ψ must be zero for all points outside the potential well. In order to keep the wave function as continuous we take $\psi=0$ at $x=0$ and at $x=L$.
Applying the first condition in eqn(3)

$$0=A\sin 0+B\cos 0=0+B \quad \text{or } B=0$$

The solution reduces to $\psi = A\sin kx \quad ---(4)$
On applying second condition in eqn(4)

$$0=A\sin kL,\ \text{since } A\neq 0;\ \sin kL=0. \quad \text{i.e } kL=n\pi, \text{ where n is an integer.}$$
$$(n=1,2,3,4,---)$$

So the solution become

$$\psi = A\sin\left(\frac{n\pi x}{L}\right) \quad ---(5)$$

We shall now evaluate the constant A by applying normalization condition for the wave function.

$$\int_0^L |\psi|^2\,dx=1. \text{ i.e. } \int_0^L A^2\sin^2\left(\frac{n\pi x}{L}\right)dx=1$$

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

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

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

$$\int_0^L\cos\left(\frac{2n\pi x}{L}\right)dx=\left[\frac{\sin\left(\frac{2n\pi x}{L}\right)}{\left(\frac{2n\pi}{L}\right)}\right]_0^L$$
$$=\frac{1}{\left(\frac{2n\pi}{L}\right)}\left[\sin\left(\frac{2n\pi L}{L}\right)-\sin\left(\frac{2n\pi\times 0}{L}\right)\right]$$
$$=0$$

Here $\int_0^L\cos\left(\frac{2n\pi x}{L}\right)dx=0$ or $\frac{A^2}{2}\int_0^L dx=\frac{A^2}{2}L=1$

Thus $A^2=\frac{2}{L}$ and $A=\sqrt{\frac{2}{L}}$

The **wave function** becomes $\boxed{\psi=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)} \quad ---(6)$

Where $n=1,2,3,4,---$

Note: If $n=0, \psi=0$ & $|\psi|^2=0$ for all values of x. so $n=0$ is ruled out.

<u>Energy Eigen values</u> (allowed energy levels):

We have $k^2 = \frac{2mE}{\hbar^2}$ and also $k = \frac{n\pi}{L}$

Or $\frac{n^2\pi^2}{L^2} = \frac{2mE}{\hbar^2}$; $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$

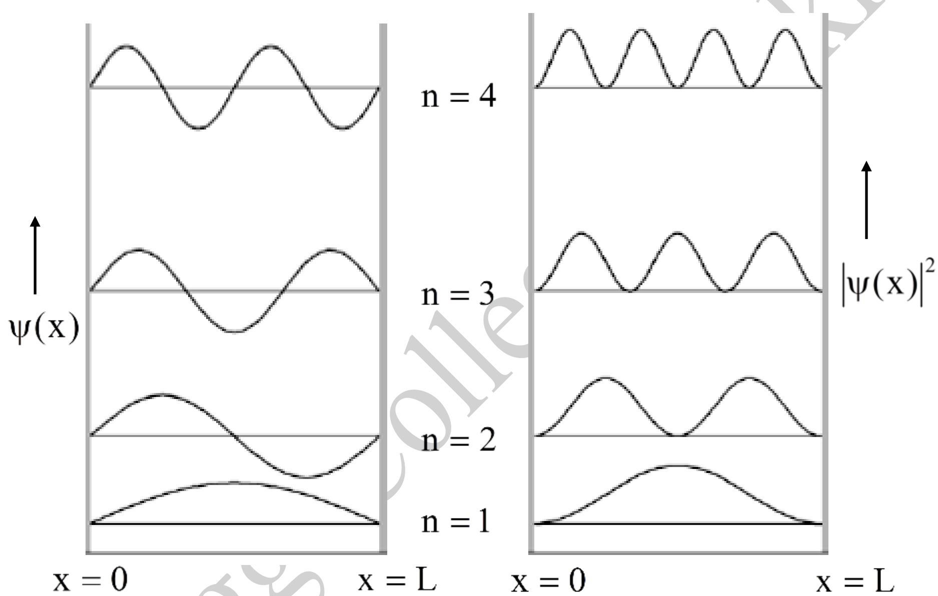
substituting for $\hbar^2 = \left(\frac{h}{2\pi}\right)^2 = \frac{h^2}{4\pi^2}$, $\boxed{E_n = \frac{n^2h^2}{8mL^2}}$ ---(7) , where $n = 1, 2, 3, 4, ---$

The different values of energy for different 'n's are called energy Eigen values. Since n is restricted, the particle does not have continuous values of energy, but restricted to certain discrete values.

<u>Eigen Functions</u>:

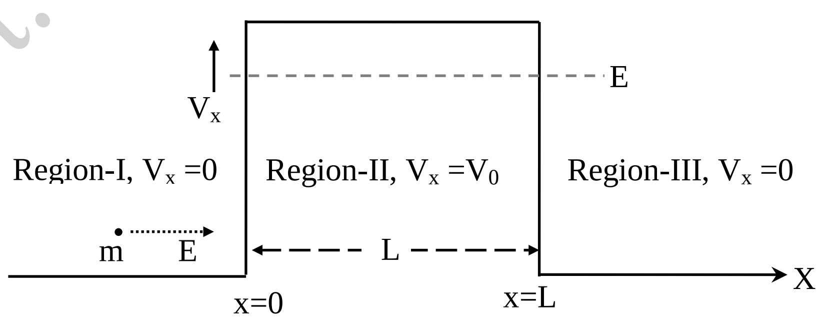
The wave functions associated with different energy eigen values are called eigen wave functions.

$$\psi_1 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) \;,\; \psi_2 = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right) \;,\; \psi_3 = \sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right) \;, ---$$



2) Quantum mechanical Tunneling:

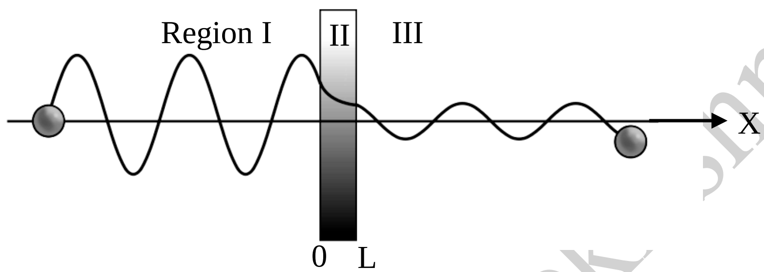
In order to understand the phenomenon of quantum mechanical tunneling, let us consider a potential barrier of height V_0 and width L as shown in the figure.



i.e, $V_x = \begin{cases} V_0 & 0 \le x \le L \\ 0 & x < 0 \text{ and } x > L \end{cases}$

According to classical mechanics, when a particle of kinetic energy E ($E < V_0$) is incident on the barrier from left, it will be reflected back without going to the other side. But in quantum mechanics there is a finite probability for the particle to be transmitted into the region III even though the energy $E < V_0$. This shows that the wave function representing the particle wave does not vanish at the barrier but penetrates through it to a certain extent. This phenomenon of **penetration (tunneling) of particles through barriers higher than their own incident energy is known as tunneling**.

The wave function during tunneling can be represented as



Schrodinger wave equation and solutions for various regions:

Region I: $\frac{\partial^2 \psi_1}{\partial x^2} + \frac{2m}{\hbar^2} E\psi_1 = 0$ (in region I, potential V=0)

$$\frac{\partial^2 \psi_1}{\partial x^2} + k_1^{\,2}\ \psi_1 = 0 \quad ---(1) \quad \text{where } k_1^{\,2} = \frac{2m}{\hbar^2} E$$

Thus wave function in region I, $\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$ $---(2)$

Here, Ae^{ik_1x} represents the incident wave and Be^{-ik_1x} represents the reflected wave in region I.

Region II: $\frac{\partial^2 \psi_2}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$ (in region II, potential $V = V_0$)

Since $V_0 > E$, we may write the equation as

$$\frac{\partial^2 \psi_2}{\partial x^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_2 = 0 \quad ; \quad \frac{\partial^2 \psi_2}{\partial x^2} - k_2^{\,2}\ \psi_2 = 0 \quad ---(3) \quad \text{where } k_2^{\,2} = \frac{2m}{\hbar^2}(V_0 - E)$$

$$\psi_2 = Ce^{k_2x} + De^{-k_2x} \quad ---(4)$$

Here, Ce^{k_2x} represents the exponentially increasing part and De^{-k_2x} represents the exponentially increasing part of the wavefunction in region II.

Region III: $\frac{\partial^2 \psi_3}{\partial x^2} + \frac{2m}{\hbar^2} E\psi_3 = 0$ (in region III, potential V=0)

$$\frac{\partial^2 \psi_3}{\partial x^2} + k_1^{\,2}\ \psi_3 = 0 \quad ---(5) \quad \text{where } k_1^{\,2} = \frac{2m}{\hbar^2} E$$

Thus wave function in region III, $\psi_3 = Fe^{ik_1x} + Ge^{-ik_1x}$ $---(6)$

As there is no reflected wave in region III, Ge^{-ik_1x} is zero and Fe^{ik_1x} represents the transmitted wave in region III. Thus $\psi_3 = Fe^{ik_1x}$

Transmission probability, $T = \frac{FF^*}{AA^*} = \frac{|F|^2}{|A|^2} = e^{-2k_2L} = e^{-\frac{2L}{\hbar}\sqrt{2m(V_0 - E)}}$ $---(7)$.