

MODULE 2- QUANTUM MECHANICS

Wave particle dualism - de-Broglie's hypothesis:

Louis de-Broglie extended the wave particle duality of light to all the fundamental entities of physics such as electrons, protons neutrons etc. de-Broglie put a bold suggestion that the wave particle dualism need not be special feature of light alone but material particles must also exhibit dual behavior. His suggestion was based on the fact that “**nature loves symmetry**”, if radiation can behave as particle under certain circumstances then, one can even expect that entities which ordinarily behave as particles to exhibit wave properties under appropriate circumstances.

According to de-Broglie's hypothesis, every moving material particle is associated with a wave whose wavelength is given by $\lambda = \frac{h}{mv} = \frac{h}{p}$, where p is the momentum of the particle.

The wave associated with moving material particle is called **matter waves** or de-Broglie waves. λ is called de-Broglie wavelength.

The expression of the wavelength associated with a material particle can be derived on the analogy of radiation as follows:

Considering the Plank's theory of radiation, the energy of a photon (quanta) is given by

$$E = \frac{hc}{\lambda}$$

And according to Einstein's mass energy relation, we have

$$E = mc^2$$

Equating above two equations, we get

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

Where c is the velocity of light and

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

Thus, wavelength of a photon is therefore specified by its momentum according to the relation

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

This equation is completely general one that applies equally well to the material particles as well as photons. The momentum of a particle of mass 'm' and velocity 'v' is $p = mv$ and its de-Broglie wavelength is accordingly

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

This physically means that a material particle of mass 'm' moving with the velocity 'v' has a wave associated with it of de-Broglie wavelength.

If E is the kinetic energy of the particle, then

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

$$\text{or } p = \sqrt{(2mE)}$$

$$\therefore \text{de-Broglie wavelength } \lambda = \frac{h}{\sqrt{2mE}}$$

$$\text{de-Broglie wavelength of an accelerated electron } \lambda = \frac{1.226}{\sqrt{V}} \text{ nm}$$

Properties of matter waves

Following are properties of matter waves:

1. Lighter is the particle, longer will be the wavelength of matter waves associated with it, velocity being constant.
2. Smaller the velocity of the particle, longer will be the wavelength of the matter waves associated with it.
3. When the particle is at rest, the wavelength associated with it becomes infinite.
i.e, when $v=0$ then $\lambda=\infty$ i.e, wave becomes indeterminate. This shows that only the moving particle produces the matter waves.
4. Matter waves are produced, whether the particles are charged or uncharged. But e. m. waves are produced by the motion of charged particle. This fact reveals that, matter waves are not electromagnetic waves.
5. The velocity of matter waves depends on velocity of material particle and it is not constant, while velocity of e. m. waves is constant.
6. Matter waves can travel even in vacuum; hence they are not mechanical waves.
7. Matter waves are represented by a wave packet made up of a group of waves of slightly different wavelengths. Hence, we talk of group velocity of matter waves rather than the phase velocity. The group velocity can be shown to be equal to the particle velocity.
8. Matter waves show properties similar to other waves such as interference and diffraction.

Phase velocity and group velocity of matter waves:

A moving material particle may be represented by de Broglie wave. The amplitude of the de Broglie wave is related to the probability of finding the particle at a particular position at a particular time. Hence we can not describe the de Broglie wave with a simple wave equation of the type $y = A \sin (wt - kx)$. Instead, one can use an equation representing a group of waves.

According to Schrodinger a moving is not equivalent to single wave, but it can be represented by **wave packet**. A wave packet is formed due to superposition of two or more individual waves each with slightly different wavelengths. The resultant pattern emerges in the shape of variation in amplitude. Such variation represents the wave group as a whole, and is called the wave packet. The velocity with which the wave packet move is called the **group velocity**.

A wave is represented by the formula

$$y = A \sin (wt - kx)$$

where y is the displacement at any instant t , a is the amplitude of vibration, w is the angular frequency ($= 2\pi\nu$) and k is the wave vector/wave number ($= 2\pi/\lambda$). The phase velocity of such a wave is the velocity with which a particular phase point of the wave travels. This corresponds to the phase being constant.

$$(wt - kx) = \text{constant}$$

$$\frac{d}{dt}(wt - kx) = 0 \quad \text{OR} \quad w - k\left(\frac{dx}{dt}\right) = 0 \quad \text{OR} \quad \frac{dx}{dt} = \frac{w}{k}$$

The phase velocity for the wave is given by $v_{\text{phase}} = \frac{w}{k}$ (1)

“If a point is imagined to be marked on a travelling wave, then it becomes a representative point for a particular phase of the wave, and the velocity with which it is transported owing to the motion of the wave, is called **phase velocity**”

In other words *the phase velocity is the velocity with which plane progressive wave travel with constant phase angle.*

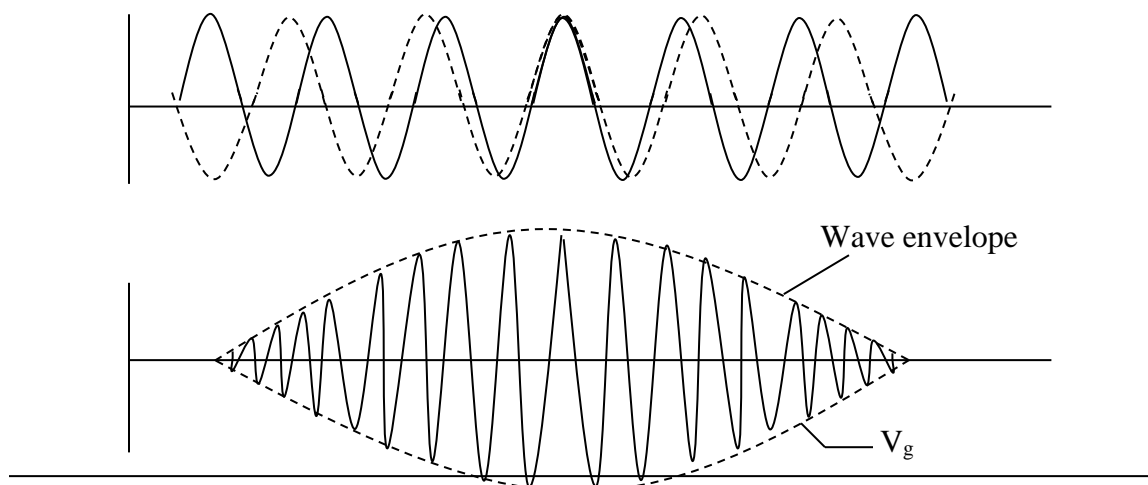
The de Broglie waves are represented by a wave packet and hence we have ‘group velocity’ associated with them. Group velocity is the velocity with which the wave packet travels. A wave packet is formed due to the superposition of two or more waves with slightly wavelength.

$$v_{\text{group}} = \frac{dw}{dk} \quad (2)$$

rate of change of the displacement of phase points in the direction of propagation with constant phase angle.

In other words *the phase velocity is the velocity with which plane progressive waves travel with constant phase angle.*

Mathematically the wave packet is the superposition of plane waves slightly differing in frequencies such that they interfere constructively over a small region of space where the particle can be located and outside this space they interfere destructively so that the amplitude reduces to zero. The rate of change of displacement of wave envelope is called group velocity.



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Figure : The super position of phase waves of nearly equal wavelengths to give the wave packet.

Heisenberg's Uncertainty principle:

The concept of dual nature of matter has a great impact on the accuracy of measurements of micro particles. To regard a moving particle as a wave group implies that there are fundamental limits to the accuracy with which we can measure particle properties such as position and momentum. In classical mechanics, a moving particle at any instant has a fixed position in space and definite momentum, which can be precisely determined if their initial values and the force acting upon it are known. However, in quantum mechanics the moving material particle is described in terms of wave packet or wave group. Hence, there are fundamental limits to the accuracy with which we can measure particle properties such as position and momentum.

Since moving material particle is regarded as de Broglie wave group, there is a limit to the accuracy with which we can measure its particle properties such as position and momentum. According to Born's probability theory the particle may be found anywhere within the wave packet. This means that position of the particle is uncertain within the limits (Δx) of the of the wave packet.

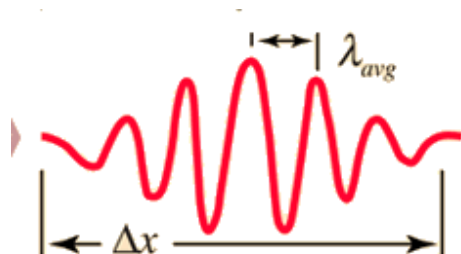
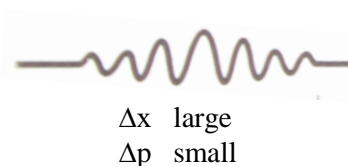
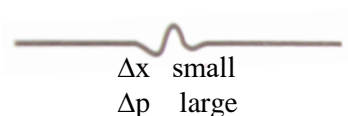


Fig. 1 wave packet

The narrower the wave group, the more precisely the particle's position can be specified. However the wavelength of the waves in narrow wave packet is not well defined; there are not enough waves to measure the ' λ ' accurately. This means that the particle momentum is not a precise quantity (because $\lambda = h/p$).

On the other hand, a wide wave group clearly defines the wavelength. Therefore the momentum corresponding to that wavelength will be a precise quantity but there is large indefiniteness in the position of the particle. This shows that it is impossible to know where within the packet the particle is located and what its exact momentum is. That is to say there is uncertainty in the measurement of position of a particle and also its momentum.



This situation is expressed in a statement by a German physicist Heisenberg which is known as Heisenberg's uncertainty principle. It states that **"it is impossible to measure precisely and simultaneously the position and momentum of an object"**

Quantitative relation:

It can also be stated as “the product of uncertainties involved in simultaneous determination of position and momentum of a particle is equal or greater than $(h/4\pi)$ ”

Mathematically Heisenberg’s uncertainty principle (HUP) can be expressed as,

$$\Delta p \cdot \Delta x \geq \frac{h}{4\pi}$$

Where Δp denotes the uncertainty (error) in the measurement of momentum and Δx is the uncertainty (error) involved in the measurement of position of the particle along x-axis, h is the Planck’s constant.

The relation is universal and holds good for energy and time also. The energy of the particle is given by

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

$$\Delta E = \frac{1}{2} m 2v \Delta v$$

$$\Delta E = m v \Delta v$$

$$= \frac{\Delta x}{\Delta t} \cdot \Delta p$$

$$\Delta E \Delta t = \Delta x \Delta p$$

$$\Delta E \Delta t \geq \frac{h}{4\pi}$$

Another form of the uncertainty principle is $\Delta L \Delta \theta \geq \frac{h}{4\pi}$; where ΔL is the uncertainty in the angular momentum and $\Delta \theta$ is the uncertainty in the angular displacement.

Uncertainties involved in the measurements are inherent in nature and not due to inaccuracy of the measuring instruments. This arises from wave properties of the material particles.

Physical significance of Heisenberg’s uncertainty principle:

Uncertainty principle places a limit on the accuracy with which the momentum and position (pair of physical variables, in general) of a particle can be measured simultaneously. The Physical Significance of this principle is that one should not think of exact position, or an accurate value for momentum of a particle. Instead one should think of the probability of finding the particle at a certain position, or of the probable value for the momentum of the particle. The estimation of such probabilities is made by means of certain mathematical function called wave function in quantum mechanics.

Application of uncertainty principle:

The non-existence of electron in the nucleus:

We can use the uncertainty principle to place a lower limit on the energy of an electron must have, if it is to be part of the nucleus.

Let us consider a typical atomic nucleus with diameter of the order of 10^{-14} m. If the electron is confined in the nucleus, then the uncertainty in the position is of the order of diameter.

$$\text{i.e } \Delta x \leq 10^{-14} \text{ m}$$

Using Heisenberg Uncertainty Principle

$$\Delta p \geq \frac{h}{4\pi\Delta x}$$

using Δx in this eqn, we get

$$\begin{aligned}\Delta p &\geq \frac{6.6 \times 10^{-34}}{4\pi (10^{-14})} \\ \Delta p &\geq 5.26 \times 10^{-21} \text{ kgm/s}\end{aligned}$$

If this is the minimum uncertainty in the momentum, then momentum p must be at least comparable to Δp .

$$\therefore p = 5.26 \times 10^{-21} \text{ kgm/s}$$

The minimum energy of electron with such a momentum we can find using eqn.

$$\begin{aligned}E &= \frac{p^2}{2m} \\ &= \frac{(5.26 \times 10^{-21})^2}{(2 \times 9.1 \times 10^{-31})} \\ &= 1.532 \times 10^{-11} \text{ J} \\ &= 95.73 \text{ MeV}\end{aligned}$$

This shows that K.E of the electron must exceed 95.73 MeV, if it is to be part of the nucleus. But experiments on beta decay show that even the electrons associated with unstable atom have a maximum energy of the order of 3-4 MeV and hence we conclude that nuclei do not contain the electrons.

Principle of Complementarity:

In physics, complementarity is a conceptual aspect of quantum mechanics that Niels Bohr regarded as an essential feature of the theory. The complementarity principle holds that objects have certain pairs of complementary properties which cannot all be observed or measured simultaneously. An example of such a pair is position and momentum. Bohr considered one of the foundational truths of quantum mechanics to be the fact that setting up an experiment to measure one quantity of a pair, for instance the position of an electron, excludes the possibility of measuring the other, yet understanding both experiments is necessary to characterize the object under study. In Bohr's view, the behavior of atomic and subatomic objects cannot be separated from the measuring instruments that create the context in which the measured objects behave. Consequently, there is no "single picture" that unifies the results obtained in these different experimental contexts, and only the "totality of the phenomena" together can provide a completely informative description.

Wave function:

In the case of electromagnetic waves, the electric and magnetic fields vary with space and time. In case of sound waves, it describes pressure variation in space and time. In analogy with these, to describe the matter waves associated with the particle motion, one requires a quantity which varies with space and time, this variable quantity is called as wave function $\psi(x, t)$.

We know that matter exhibits wave like behavior under certain conditions. When the momentum of the particle is well defined, the wave can be of infinite extent. Therefore a particle moving along x-axis with well-defined momentum is described by an infinite plane wave $\psi(x, t)$ and is given by

$$\psi(x, t) = Ae^{i(kx - \omega t)}$$

It is a function of space variables (x, y, z) and time 't', where ω is angular velocity and k is wave vector.

Physical significance of wave function:

1. The wave function Ψ provides all possible information about the particle which is associated with wave-character. The state of the system is described or represented by Ψ which is a function of space and time coordinates.
2. It is a complex quantity representing the matter wave associated with moving particle.
3. It is large in magnitude where the particle is likely to be located and small in other places.
4. It connects the particle nature and its associated wave nature.
5. The wave function Ψ has no direct physical meaning. But square of absolute value of wave function $|\Psi|^2$ has physical significance. $|\Psi|^2$ is a measure of the probability of finding the particle at a particular position. It does not give the exact location of the particle.

Probability density:

The probability density of a particle associated with de-Broglie waves can be represented as $P = \Psi\Psi^* = |\Psi|^2$ where ψ is wave function & ψ^* is the complex conjugate of ψ . $|\Psi|^2 = \Psi^*\Psi$ is real and positive and has physical meaning.

(Probability of occurrence of an event is a real and positive quantity but wave function may be complex. Hence in order to get a real and +ve value while evaluating $|\Psi|^2$, the wave function is ψ is multiplied with its complex conjugate Ψ^)

Consider a particle is in a volume V inside which particle is known to be present in a volume element dV. Let Ψ be the wave function associated with the particle then the square of the wave function associated with the particle is interpreted as measure of probability density. That is $|\Psi|^2$ is the probability density per volume element and the particle will be found in that volume element

Normalization of wave function:

Let V be a volume inside which a particle is known to be present, but where exactly the particle is situated in V is not known. Then the probability of finding the particle in a volume element dV is expressed as

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

Since $|\psi|^2 dV$ is the probability that the particle will be found in a volume element dV , the total probability that the particle will be somewhere in the space must be equal to unity. Thus we have

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

The normalizing condition for the wave function for the motion of a particle in one dimension is

$$P = \int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

The above condition is called **normalization condition**. A wave function which satisfies above equation is said to be normalized.

Normalization is simply a statement that the particle exists at some point at all the times. Therefore, although it is not possible to specify the position of the particle with complete certainty, it is possible to specify only the probability of observing it. Thus it turns out that the waves have no real material characteristics, but are purely a measure of probability.

Properties of wave function:

Besides being normalizable, the wave function ψ must satisfy the following properties

1. Ψ must be single valued.
2. Ψ must be finite everywhere.
3. Ψ and its first derivatives $d\Psi/dx$, $d\Psi/dy$ and $d\Psi/dz$ must be continuous.
4. For bound states, Ψ or if Ψ is complex then $\Psi^* \Psi$ must vanish at infinity.

The wave functions which are finite, continuous, single valued and normalized are called **Eigen functions**.

Equation of motion for de-Broglie waves:

Schrodinger in the year 1925 formulated the wave equation which is known as the Schrödinger equation of motion to describe the wave nature of a particle based on de Broglie's ideas of matter waves. This equation cannot be derived from any fundamental laws. It is the fundamental equation of quantum mechanics in the same sense that the second law of motion ($F = m d^2x/dt^2$) is the fundamental equation of Newtonian mechanics. It is the wave equation in the variable Ψ called wave function. There are two wave equations namely

1. Schrodinger time independent wave equation
2. Schrodinger time dependent wave equation

These equations are used to determine the electron energy levels in atoms and molecules. They also enable to find the location or state of the electron in a material.

Schrödinger time independent wave equation:

In many cases the potential energy V of the particle does not depend on the time t explicitly. The forces that act on the particle and hence potential energy vary with the position of the particle only. The wave equation describing only the position of the particle is called time independent Schrodinger wave equation.

Consider one dimensional wave function Ψ describing the de Broglie wave for a particle moving freely in the positive X-direction. Ψ be the wave function which represents the displacement of the particle moving with velocity ' v ' at any time ' t '.

$$\psi(x, t) = Ae^{i(kx - \omega t)} \quad (1)$$

where A is the wave amplitude

k is the wave vector

ω is the angular frequency

Differentiating equation (1) twice w. r. to ' t ' we get

$$\begin{aligned} \frac{d\psi}{dt} &= Ae^{i(kx - \omega t)} (-i\omega) \\ \frac{d^2\psi}{dt^2} &= Ae^{i(kx - \omega t)} (-\omega)^2 \\ &= -(\omega)^2 \psi \end{aligned} \quad (2)$$

In general, classical differential equation for plane progressive wave is given by

$$\frac{d^2y}{dx^2} = \frac{1}{v^2} \frac{d^2y}{dt^2}$$

In analogy to above equation we can write the wave equation of de-Broglie waves by replacing y by Ψ

$$\frac{d^2\psi}{dx^2} = \frac{1}{v^2} \frac{d^2\psi}{dt^2} \quad (3)$$

Substitute equation (2) in equation (3)

$$\begin{aligned} \frac{d^2\psi}{dx^2} &= -\frac{1}{v^2} (\omega)^2 \psi \\ \frac{d^2\psi}{dx^2} &= -\frac{\omega^2}{v^2} \psi \end{aligned} \quad (4)$$

We have, $\omega = 2\pi\nu$, $v = \nu\lambda$

Substitute ω and v in equation (4)

$$\frac{d^2\psi}{dx^2} = -\frac{(2\pi\nu)^2}{(\nu\lambda)^2} \psi = -\frac{4\pi^2\nu^2}{\nu^2\lambda^2} \psi = -\frac{4\pi^2}{\lambda^2} \psi \quad (5)$$

For a particle of mass ' m ' and velocity ' v '

$$\begin{aligned} \lambda &= \frac{h}{p} = \frac{h}{mv} \\ \therefore \frac{d^2\psi}{dx^2} &= -\frac{4\pi^2 m^2 v^2}{h^2} \psi \end{aligned} \quad (6)$$

But, Total Energy $E = K.E + V$

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

$$(\text{or}) E - V = \frac{1}{2}mv^2$$

$$(\text{or}) m^2v^2 = 2m(E - V)$$

Substituting in Equn. (6) and rearranging, we get

$$\therefore \frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2}(E - V)\psi = 0$$

This is Schrödinger wave equation for a particle in one dimension case.

For 3 – dimensional case

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2m(E - V)}{h^2}\psi = 0$$

Expectation value:

To relate a quantum mechanical calculation to something you can observe in the laboratory, the "expectation value" of the measurable parameter is calculated. For the position x , the expectation value is defined as

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x,t)x\psi(x,t)dx$$

This integral can be interpreted as the average value of x that we would expect to obtain from a large number of measurements. Alternatively it could be viewed as the average value of position for a large number of particles which are described by the same wave function. For example, the expectation value of the radius of the electron in the ground state of the hydrogen atom is the average value you expect to obtain from making the measurement for a large number of hydrogen atoms.

While the expectation value of a function of position has the appearance of an average of the function, the expectation value of momentum involves the representation of momentum as a quantum mechanical operator.

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x,t) dx$$

where

$$p_{operator} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

is the operator for the x component of momentum.

Since the energy of a free particle is given by

$$E = \frac{p^2}{2m} \quad \text{then} \quad \langle E \rangle = \frac{\langle p^2 \rangle}{2m}$$

and the expectation value for energy becomes

$$\langle E \rangle_{free\ particle} = \int_{-\infty}^{\infty} \psi^* \frac{(-\hbar^2)}{2m} \frac{\partial^2}{\partial x^2} \psi dx$$

for a particle in one dimension.

In general, the expectation value for any observable quantity is found by putting the quantum mechanical operator for that observable in the integral of the wave function over space:

$$\langle Q \rangle = \int_{-\infty}^{\infty} \psi^* Q_{operator} \psi dV$$

integral over
all space

Eigen functions and Eigen values:

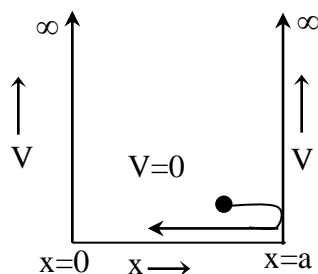
A system is defined by its energy, momentum, position etc. Once, the wave function corresponding to system is known, the state of the system can be determined. In order to find Ψ , the Schrödinger equation has to be solved. But, it is second order differential equation; there are not one but several solutions. All of them may not be correct wave functions which we are looking for. We have to select those wave functions which would correspond meaningfully to a physical system. Such acceptable well behaved wave functions which are finite, continuous, single valued and normalized are called **eigen functions** while the energies corresponding to these eigen functions are called **eigen values**. (*Eigen is the German word meaning proper or characteristic*).

Applications of Schrödinger wave equation:

1. Particle in a one dimensional potential well of infinite height (or particle in a box):

The simplest quantum mechanical problem is that of the particle trapped in a box of infinitely hard walls. Consider a particle of mass m is free to move in x -direction only. We may specify a particle motion by saying that it is restricted to travel along the x -axis between $x=0$ to $x=a$ by infinitely hard walls. The particle makes elastic collisions with walls so its total energy remains constant. From a formal point of view consider potential $V = \infty$ on the both the side of the box and say $V = 0$ inside the box. Because the particle can't have infinite energy it can't exist outside the box, so $\psi = 0$ for $x \leq 0$ and $x \geq a$

$$\begin{aligned} \text{i.e. } V(x) &= \infty & \text{for } x \leq 0 \text{ and } x \geq a \\ \text{and } V(x) &= 0 & \text{for } 0 < x < a \end{aligned}$$



The Schrödinger wave equation for wave like particle is given by

$$\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2m}{h^2}(E - V)\psi(x) = 0$$

Out side the box (for $V=\infty$), the Schrödinger equation becomes

$$\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2m}{h^2}(E - \infty)\psi(x) = 0$$

This equation holds good only if $\Psi=0$ for all points outside the box i.e., $|\Psi|^2 = 0$, probability of finding the particle outside the box is zero.(or particle cannot be found at all outside the box)

Inside the box ($V=0$), the Schrödinger equation becomes

$$\frac{d^2\Psi(x)}{dx^2} + \frac{8\pi^2m}{h^2}E\Psi(x) = 0$$

$$\text{(or)} \quad \frac{d^2\Psi(x)}{dx^2} + k^2\Psi(x) = 0 \quad (1)$$

$$\text{where } k = \sqrt{\frac{8\pi^2m}{h^2}E}$$

The solution of equation (1) takes the form

$$\Psi(x) = A \cos(kx) + B \sin(kx) \quad (2)$$

Where A and B are constants which can be evaluated by applying boundary conditions

(i) But, at $x = 0$, $\Psi = 0$ as per condition I

\therefore equation (2) becomes

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

$$\text{(or)} \quad A = 0 \quad (3)$$

(ii) at $x = a$, $\Psi = 0$ equation (2) becomes

$$\Psi(a) = 0 = A \cos(ka) + B \sin(ka)$$

But $A = 0$ from equation (3)

$$\therefore \Psi(a) = 0 = B \sin(ka) \quad (4)$$

Here either $B = 0$ or $\sin(ka) = 0$; but $B \neq 0$ because if $B = 0$ the entire function given by equation (2) will be zero as $A = 0$. $\Psi = 0$ leads to no probability of finding the particle, but we are dealing with the particle present in the potential well, thus equation (4) is satisfied only when

$$\sin(ka) = 0$$

$$\text{(or)} \quad ka = n\pi$$

$$\therefore \sin n\pi = 0 \text{ for } n = 0, 1, 2, 3, \dots$$

n is called quantum number.

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

\therefore substituting for k and B , equation (2) can be written as

$$\Psi_n(x) = B \sin \frac{n\pi}{a} x \quad (5)$$

Our solution $\Psi(x)$ is yet not complete since we have not yet determined the constant A . To do this, we use the normalization condition,

$$\int_{-\infty}^{\infty} |\Psi|^2 dx = 1,$$

Since $\Psi = 0$ except for $0 < x < a$, the integral vanishes except inside that region, so that

$$\int_0^a B^2 \sin^2 \frac{n\pi x}{a} dx = 1,$$

but $\sin^2 \theta = \frac{1}{2} (1 - \cos 2\theta)$

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

$$\therefore \frac{B^2}{2} \left[x - \frac{a}{2n\pi} \sin \left(\frac{2n\pi x}{a} \right) \right]_0^a = 1$$

$$\Rightarrow \frac{B^2}{2} \left[a - \frac{a}{2n\pi} \sin \left(\frac{2n\pi a}{a} \right) - 0 \right] = 1$$

$$\Rightarrow \frac{B^2}{2} [a] = 1 \quad (\because \sin 2n\pi = 0)$$

$$\therefore B = \sqrt{\frac{2}{a}}$$

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

which represents the permitted solution.

Eigen value:

Using equation $k = \sqrt{\frac{8\pi^2 m}{h^2}} E$ and $k = \frac{n\pi}{a}$

$$\frac{n\pi}{a} = \sqrt{\frac{8\pi^2 m}{h^2}} E$$

$$\left(\frac{n\pi}{a} \right)^2 \times \frac{h^2}{8\pi^2 m} = E$$

$$E_n = \frac{n^2 h^2}{8ma^2} = n^2 E_0$$

Where $n=1,2,3,\dots$ and $E_0 = \frac{h^2}{8ma^2}$ is called **zero point energy**.

From above equation it is clear that the energy of the particle can have only certain values i.e., energy of the particle is quantized.

Below is represented a schematic diagram of wave functions energy values and probability density Ψ^2 for the first three permitted states.

Case (i) : For $n=1$

This is the ground state and normally particle is found in this state.

$$E_1 = h^2 / 8ma^2$$

And $\psi_1 = (2/a)^{1/2} \sin(\pi x/a)$
 with $\psi_1 = 0$ at $x = 0$ and $x = a$
 But ψ_1 is maximum at $x = a/2$.

Case (ii) : For $n=2$

This is the first excited state.

$$E = 4h^2/8ma^2 = 4 E_0$$

And $\psi_2 = (2/a)^{1/2} \sin(2\pi x/a)$

with $\psi_2 = 0$ at $x = 0, a/2$ and a

and ψ_2 reaches maximum values for $x = a/4$ and $3a/4$.

Case (iii): For $n=3$

This is the second excited state.

$$E = 9h^2/8ma^2 = 9 E_0$$

And $\psi_3 = (2/a)^{1/2} \sin(3\pi x/a)$

with $\psi_3 = 0$ at $x = 0, a/3, 2a/3$ and a

and ψ_3 reaches maximum values for $x = a/6, a/2$ and $5a/6$.

