Module 3
Elementary Quantum Mechanics & Application of Quantum Mechanics

Lecture 1

1.1 Historical Overview

In the middle of the 19th and 20th century, it was believed that Newtonian physics and thermodynamics are well enough to explain all the phenomena in nature. Basically, during that time Newton's laws successfully describes the dynamics of particles and Maxwell's equations describes the electromagnetic fields phenomena. Further, classical mechanics suitably explains the motion of celestial bodies like planets, stars, macroscopic and terrestrial bodies moving with non-relativistic speeds. However, classical theory does not hold in the region of atomic dimensions, i.e., it cannot explain the non-relativistic motion of electrons, protons etc. Thus, failure of classical mechanics to explain necessitates the development of new physics i.e., *Quantum Physics* to explain atomic dimension systems.

The shortcoming of Classical physics is as follows:

➢ It could not explain the stability of atoms.
➢ It does not hold in the region of atomic dimensions.
➢ It could not explain the observed spectrum of blackbody radiation.
➢ It could not explain the observed variation of specific heat of metals and gases.
➢ It could not explain the origin of discrete spectra of atoms

Although classical physics fails to explain a large number of observed phenomena such as photoelectric effect, Compton Effect, Black body radiation, etc. The most significant is the consideration of *continuous distribution of energy*. Basically, at the microscopic level (in the region of atomic or subatomic level) the concept for interpretation of energy distribution is discrete rather than continuous. This module facilitates to learn and understand basic concepts of quantum mechanics such as wave-particle duality, de-Broglie waves and Heisenberg principle, Wave function and Schrödinger wave equation and its applications.

1.2 Matter Waves

❖ It is well understood from various experiments such as photoelectric effect, Newton's ring experiment, etc. that light, the electromagnetic radiation, possesses dual character of a particle as well as a wave. The wave- particle duality is only the concept of energy

transmission of radiation and radiation sometimes behaves as particle nature and sometimes as wave and both cannot be separated.

❖ In 1924, de-Broglie proposed that wave particle duality is not only associated with radiation, but matter such as *electron, proton, neutron*, etc. also possess this dualism characteristic. Therefore, a wave is always associated with the moving particle whether it is matter or radiation and controls the particle.

❖ The occurrence of properties of wave or particle depends upon the conditions under which the particular phenomenon takes place; however, both particle and wave cannot appear together.

1.2.1 de-Broglie hypothesis

According to de-Broglie hypothesis, a particle in motion always has a wave associated with it and the motion of the particle is guided by that wave. These waves are called de-Broglie waves or matter waves. The wavelength λ of matter waves associated with a moving particle is given by:

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2mK}} \quad \text{(For non-relativistic particle)}$$

Where, p is the momentum, m is the mass, v is velocity and K is the kinetic energy of the particle. This relation is true when v<<c. This wavelength is known as de-Broglie wavelength.

• If a charged particle having charge q is accelerated through a potential difference of V volts then de-Broglie wave is.

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2qmV}} \quad [E=qV]$$

• According to kinetic theory of gases, the average kinetic energy of material particle is given by

$$E = \frac{1}{2}mv^2 = \frac{3}{2}kT$$

The de-Broglie wavelength associated with the gaseous particles will be:

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{3mKT}}$$

• Similarly, for a relativistic particle the de-Broglie wavelength can be obtained as:

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$$E = p^2 c^2 + m_o{}^2 c^4$$

$$p = \frac{\sqrt{E^2 - m_o{}^2 c^4}}{c} \; ; \lambda = \frac{h}{p} = \frac{hc}{\sqrt{E^2 - m_o{}^2 c^4}}$$

Lecture 2

1.3 Heisenberg's Uncertainty Principle

❖ Heisenberg in 1927 proposed an uncertainty principle which was direct consequence of dual nature of matter. It is well known that in classical mechanics a particle is described by its definite momentum (velocity) and position. Therefore, its position and velocity (momentum) both can be determined with desired accuracy.

❖ However, in quantum mechanics a particle is described by a wave packet moving with group velocity and particle can be located anywhere within the limit of wave packet. Therefore, position of particle in the packet is not certain.

Definition: *Heisenberg's uncertainty principle can be defined as it is impossible to determine the exact position and momentum of a particle simultaneously.*

Mathematically, uncertainty principle can be defined as the product of uncertainty in determining the position and momentum of a particle at the same instant is greater than or equal to $\frac{\hbar}{2}$; where $\hbar = \frac{h}{2\pi}$;

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

Where, Δx : Uncertainty in determining position x, Δp_x : Uncertainty in determining x-component of momentum.
Another useful form of the uncertainty principle relates energy and time:

$$\textbf{i.e.,} \; \Delta E . \Delta t \geq \frac{\hbar}{2}.$$

This form uncertainty indicates that it is not possible to determine both the energy and time co-ordinate of a particle with unlimited precision.

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1.3.1 Physical Significance of Heisenberg's Uncertainty Principle

❖ If one can measure the position 'x' of a particle, then uncertainty in position 'Δx' vanishes while uncertainty in momentum becomes infinite and vice-versa. Thus, if an experiment will be designed to measure 'x' or 'p' accurately, the other quantity will become completely uncertain.

❖ One can measure both the quantities by means of experiment but only to a certain limit of accuracy specified by the uncertainty principle.

❖ Classical mechanics is true for heavy bodies, and the uncertainties are characteristics of quantum mechanics which is applicable to light particles such as electron, proton, neutron etc.

1.4 Applications of Uncertainty Principle
1.4.1. Non-existence of free electron in nucleus

Let us assume that the electron is present inside the nucleus whose diameter is typically of the order of 10^{-14} m. Therefore, the maximum uncertainty in the position of electron is nothing but the diameter of the nucleus, that is, $\Delta x = 10^{-14} m$.

Then, according to uncertainty principle, the uncertainty in momentum is given by:

$$\Delta p_{min} = \frac{\hbar}{\Delta x_{max}}$$

Therefore, minimum uncertainty in momentum will be:

$$\Delta p_{min} = \frac{\hbar}{\Delta x_{max}} = \frac{6.62 \times 10^{-34}}{6.28 \times 10^{-14}} = 1.05 \times 10^{-20} kgm/\sec$$

Further, minimum uncertainty in momentum physically means momentum itself, that is, $\Delta p_{min} = p$. Thus, the total relativistic energy of a particle is given by:

$$E = \sqrt{p^2 c^2 + m_o^2 c^4}$$

As the rest mass energy of an electron is only 0.51 MeV, which is very small and hence can be neglected, therefore,

$$E = pc = 1.05 \times 10^{-20} kg \ m/s \ \times \ 3 \times 10^{8} m/s = 3.15 \times 10^{-12} J = 19.6 MeV$$

Thus, if a free electron exists inside the nucleus, it must have a minimum energy of about 19.6 *MeV*, but experiments shows that the electron emitted from a radioactive nucleus can have a maximum energy of about *1 MeV.* Therefore, it can be concluded that a free electron cannot exist inside the nucleus.

Lecture 3

1.5 Wave Functions

❖ Waves in general are associated with quantities that vary periodically. In case of matter waves, the quantity that varies periodically is called *wave function.*A wave function, represented by **ψ**, associated with the matter waves has no direct physical significance. However, the value of the wave function is related to the probability of finding the particle at a given place at a given time.

❖ The square of the absolute magnitude of the wave function of a body evaluated at a particular time at a particular place is proportional to the probability of finding the particle at that place at that instant.

❖ The wave functions are usually complex and the probability in such a case is taken as $\psi * \psi$, i.e., the product of the wave function with its complex conjugate $\psi *$. Since the probability of finding a particle somewhere is finite, the total probability over all space equal to unity i.e.,

$$\int_{-\infty}^{\infty} \psi * \psi dV = 1 \ \text{or} \ \int |\psi(r,t)|^{2} d\tau = 1$$

Where, $dV = dxdydz$. The above equation is called the *normalization condition* and a wave function that obeys this equation is said to be *normalized*.

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1.5.1 Orthonormal Condition:

Orthogonal + Normalized function

$$\int_{-\infty}^{\infty} \psi_i * \psi_j d\tau = 1, when\ i = j$$
$$= 0\ when\ i \neq j$$

1.5.2 Significance of Wave Functions

Apart from being normalizable, a well-behaved or acceptable wave function must fulfill the following conditions:

➢ ***The wave function ψ must be finite everywhere***: If ψ is infinite at a particular point then it means that there is an infinitely larger probability of finding the particle at that particular point which is clear violation of uncertainty principle.

➢ **The wave function ψ must be single valued:** If ψ has more than one values at a particular point then it means there is more than one value of probability of finding the particle at that particular point, which is not possible.

➢ The wave function ψ must be continuous and must have continuous first-order derivative everywhere: If $\frac{d\psi}{dx}$ is continuous then, ψ will obviously be continuous.

Lecture 4

1.6 Eigen Value and Eigen Functions

If an operator $(\hat{A})$ operating on a function $\psi(x)$ results the same wave function $\psi(x)$ multiplied by constant (λ); then $\psi(x)$ is called *Eigen function* of $\hat{A}$ belonging to the Eigen value λ.

Mathematically, $\hat{A}\psi(x) = \lambda\psi(x)$

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Example:

$$\text{Let } \psi(x) = e^{4x} \text{ and } \hat{A} = \frac{d}{dx},$$

$$\text{Then } \hat{A} \ \psi(x) = \frac{d}{dx}\left(e^{4x}\right) = 4.e^{4x}$$

So here Eigen Function= e^{4x} and Eigen Value=4.

1.7 Expectation Value (Average value)

It is defined as the average of the large numbers of independent measurements on the same system. Expectation value of any operator (say $\hat{A}$) can be represented as :

$$\left\langle \hat{A} \right\rangle = \frac{\int \psi^* \hat{A} \psi \, dV}{\int \psi^* \psi \, dV}$$

If ψ is normalized then $\int \psi^* \psi \, dV = 1$. So, in that case: $\left\langle \hat{A} \right\rangle = \int \psi^* \hat{A} \psi \, dV$.

N.B: ψ* is the complex conjugate of ψ.

1.8 Operators

The word 'operation' means action, so an operator is an actor which can change a physical quantity having taken some action on it. Basically,*an operator is defined as a rule by which a given function is transformed into another function*.

If the operator A transforms f(x) into the function g(x), it can be written as:

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

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

1.8.1 Linear operator

If an operator A satisfies the following two properties, it is said to be a linear operator:

$$\hat{A}\left[f_1(x) + f_2(x)\right] = \hat{A} f_1(x) + \hat{A} f_1(x)$$

$$\hat{A}\left[cf(x)\right] = c\,\hat{A}f(x)$$

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Where, c is an arbitrary constant.

NB: Each dynamical variable in quantum mechanics is represented by an operator.

(a) **Cartesian co-ordinate operator**: Cartesian coordinates are $\hat{x}, \hat{y}, \hat{z}$ co-responding to x,y, z coordinates of a particle in Cartesian coordinate space. $\hat{x}\psi(x) = x\psi(x)$

(b) **Momentum Operator ($\hat{P}$)**

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

$$\frac{\partial \psi}{\partial x} = ik\psi$$

multiplying both sides by $\dfrac{\hbar}{i}$

$$\frac{\hbar}{i}\frac{\partial \psi}{\partial x} = \frac{\hbar}{i}ik\psi = \hbar k\psi.$$

$\because$ As per De Broglie hyothes is :

$$\lambda = \frac{h}{p}; \Rightarrow p = \frac{h}{\lambda} = \frac{h/2\pi}{\lambda/2\pi} \Rightarrow p = \hbar k. \quad \left(\because k = \frac{2\pi}{\lambda} \ \& \ \hbar = h/2\pi\right)$$

$$\frac{\hbar}{i}\frac{\partial \psi}{\partial x} = p\psi$$

$$\therefore p_x = \frac{\hbar}{i}\frac{\partial}{\partial x} = -i\hbar\frac{\partial}{\partial x} \quad \text{(in 1D)}$$

$$\hat{P} = -i\hbar\nabla \quad \text{(in 3D)}$$

(c) **Kinetic energy operator**

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x} = -i\hbar\frac{\partial}{\partial x}\text{(differntiating the equation)}$$

$$\frac{\hbar}{i}\frac{\partial^2\psi}{\partial x^2} = p_x\frac{\partial\psi}{\partial x}, \text{ Hence } \frac{\hbar}{i}\frac{\partial^2\psi}{\partial x^2} = p_x\cdot\left(\frac{i}{\hbar}p_x\psi\right)$$

i.e

$$p_x^2\psi = \frac{\hbar^2}{i^2}\frac{\partial^2\psi}{\partial x^2} \Rightarrow \frac{p_x^2}{2m}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}\left(\text{dividing 2m both side}\right)$$

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Now the kinetic energy can be expressed as

$$T_x = \frac{1}{2}mv^2 = \frac{1}{2}\frac{p_x^2}{m}$$

So, the above equation can be written as

$$T_x \psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \text{ in 1D; } \hat{T} = -\frac{\hbar^2}{2m}\nabla^2 \text{ (3D)}$$

(d)Potential energy operator

$$\hat{V}(x)\psi = V(x)\psi \text{ in 1D}$$

$$\hat{V}(\vec{r})\psi = V(r)\psi \text{ in 3D}$$

(e)Hamiltonian operator ($\hat{H}$)

Hamiltonian means total energy i.e. sum of kinetic and potential energy

So,
$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \text{ in 1D}$$
$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \text{ in 3D}$$

(f)Energy operator ($\hat{E}$)

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

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

$$i\hbar\frac{\partial\psi}{\partial t} = (i\hbar)(-i\omega)\psi = \hbar\omega\psi \text{ (Multiplying both sides by } i\hbar)$$

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

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

Lecture-5

1.9 Schrödinger's equation - Time dependent and time independent

In quantum mechanics any physical system is describe by a wave function Ψ(r, t), which contains all the information about the system. This wave function satisfies all the characteristics of the wave functions.

The Time Dependent Schrödinger Wave Equation

We know from the de Broglie's hypothesis particle has dual nature means particle has wave nature also. A particle of mass m moving along x-axis represented by

$$\psi(x,t) = Ae^{-i(kx-\omega t)} . \qquad \text{… L5.1}$$

Now, if we do second order differentiating with respect to *x* and first order differentiating with respect to *t*,

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi \text{ and } \frac{\partial \psi}{\partial t} = -i\omega\psi. \quad \text{…L5.2}$$

From equation (L5.2)

$$i\hbar\frac{\partial \psi}{\partial t} = \hbar\omega\psi \qquad \text{… L5.2a}$$

$$i\hbar\frac{\partial \psi}{\partial t} = \frac{\hbar^2 k^2}{2m}\psi$$

> We Know, Energy (E) can be written $E = \hbar\omega = \frac{p^2}{2\,m} = \frac{\hbar^2 k^2}{2m}$

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \quad \text{(After replacing k}^2 \text{ using equation L5.2) ……. L5.3}$$

This is the time dependent Schrödinger equation for a free particle in one dimension.

If the particle moving in a potential V(x), then total energy, $E = \frac{p^2}{2\,m} + V(x).$

So, the time dependent Schrödinger equation for a particle in a potential V in one dimension is

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi. \qquad\qquad \ldots \qquad L5.4$$

So, the time dependent Schrödinger equation for a particle in a potential V(x,y,z) in three dimension is

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

$$i\hbar\frac{\partial\psi(x,y,z,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x,y,z)\psi \qquad\qquad \ldots. \text{L5.5}$$

The Time Independent Schrödinger Wave Equation

The time independent Schrödinger equation for a particle in one dimension can be written as(from L5.2a $i\hbar\frac{\partial\psi}{\partial t} = \hbar\omega\psi = E\psi$)

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x). \qquad\qquad \ldots\text{L5.6}$$

 In three dimension,

$$E\psi(x,y,z) = -\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) \qquad \ldots\text{L5.7}$$

Lecture-6

Free Particle (Eigen values and Eigen functions)

The net external force on a particle can be written in terms of potential is $F = -\frac{dV}{dx}$. In case of free particle the potential is constant which can be chosen as zero i.e. V=0.

So the time independent Schrödinger for a free particle in one dimension moving along x axis is-

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0 \qquad\qquad \ldots\text{L6.1}$$

where, $k^2 = \dfrac{2mE}{\hbar^2}$. ...L6.2

The equation (L6.1) is second order homogeneous differential equation. The solution of the equation can be written as

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad .$$ ...L6.3

Here, A and B are the arbitrary constants. In the equation (L6.3), the first and second terms represent plane wave travelling along +x axis and –x axis, respectively.

The energy eigen value for free particle (from L6.2) is

$$E = \dfrac{\hbar^2 k^2}{2m}.$$ ... L6.4

Since there is no restriction on the values of k, the energy can take any finite values. So the energy spectrum of the free particle is **CONTINUOUS**.

Here, Ae^{ikx} and Be^{-ikx} are the Eigen function of the energy operator have same energy Eigen value $E = \dfrac{\hbar^2 k^2}{2m}$. Hence the states are **DISCRETE**.
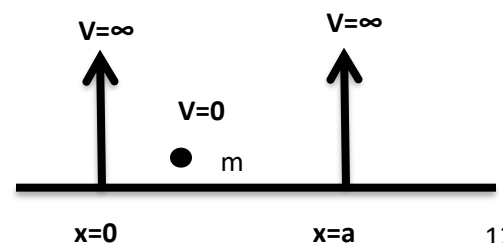
The de Broglie wave length associated with free particle is

$$\lambda = \dfrac{h}{p} = \dfrac{h}{\sqrt{2mE}} \,.$$

Lecture-7

Energy Eigen values and Eigen functions of a particle enclosed in one-dimensional potential box of infinite height or infinitely deep potential well.

Consider a particle of mass m and energy E moving along X-axis between the two rigid walls A and B at x=0 and x=a.

This means

V=∞ for x≤ 0 and x≥ a

V=0 for 0< x< a ……………………………………………………. L7.1

The particle is free to move between the walls. Since the walls are rigid and impenetrable, the probabilities of the particle to be at x=0 and x=a must be zero. Since the probability is measured by the modulus square of the wave amplitude this means that the wave function $\Psi(x)$ must be zero at x=0 and x=a. Thus

$$\Psi(0) = \Psi(a) = 0 \quad\text{……………………………………………….L7.2}$$

These are the boundary conditions. The continuity condition then requires that Ψ=0 everywhere outside the box (i.e., for x<0 and x>a).

Since the potential energy is time-dependent, we use one-dimensional time-independent Schrodinger equation for the particle,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - v)\psi = 0 \quad\text{…………………………………………….L7.3}$$

As V=0 between the walls, the above equation has the following form

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0 \; for \; 0 < x < a$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + k^2\psi(x) = 0 \quad\text{……………………….L7.4}$$

$$k^2 = \frac{2mE}{\hbar^2} \; Or \; k = \sqrt{\frac{2mE}{\hbar^2}} \quad\text{…………………}\quad \text{L7.5}$$

The general solution of equation (4) is of the form $\psi(x) = A_1 e^{ikx} + A_2 e^{-ikx}$ which can be expressed as combinations of $\sin kx$ and $\cos kx$. Thus the general solution may be given by

$$\psi(x) = A \sin kx + BCosKx \text{…………………………………………}\quad \text{L7.6}$$

Where, A and B are two constants which are to be determined from the boundary conditions. At X=0, Eqn.(6) gives $\psi(0) = A \sin(0) + BCos(0)$ or $\Psi(0) = B$. Applying the boundary condition $\psi(0) = 0,$ we have

B=0…………………………………………….L7.7

$\psi(x) = A \sin kx$ …………………………………………………………..L7.8

At $x = a,\ \psi(a) = A \sin ka$ and the boundary condition, $\psi(a) = 0\ gives, A \sin ka = 0$. Here either A=0 or $\sin ka = 0$ but A≠ 0 because if $A = 0$, the entire wave function (8) is zero (for finite values of k).

So, $\sin ka = 0\ or ka = n\pi$ (where n=1,2,3…….) …………………....L7.9

The value n=0 is excluded since this will make $\Psi = 0$ everywhere.

Energy Eigen Values

From eqn.(9), we have $k = \dfrac{n\pi}{a}$ $(n = 1,2,3, … . …)$

$$k^2 = \frac{n^2\pi^2}{a^2}$$

Using eqn.(5), we have $\dfrac{2mE}{\hbar^2} = \dfrac{n^2\pi^2}{a^2}$

(Here $\boxed{E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}}$ .10)

This is the energy Eigen value equation.

It is clear from eqn.(L7.10) that inside an infinitely deep potential well, the particle can have only discrete set of values of energy i.e., the energy of the particle is quantized. For n=1, we get ground state energy $E_1 = \dfrac{\pi^2\hbar^2}{2ma^2}$ and energy of other excited states are $E_2 = 4E_1, E_3 = 9E_1$ etc.i.e., $E_n = n^2 E_1$. Spacing between two adjacent energy levels is

$\Delta E= E_n - E_{n-1} = [n^2 - (n-1)^2]E_1 = (2n-1)E_1.$

Eigen Functions

The wave function (L7.8)by use of eqn. (L7.10), becomes

$$\psi(x) = A \sin \frac{n\pi x}{a} \quad \text{..................................} \quad \text{L7.11}$$

The constant A of eqn.L7 (11)can be obtained by applying the normalization condition

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

Or $\quad\quad \int_{-0}^{a} |\Psi|^2 dx = 1 \quad\quad (\Psi = 0 \; for x < 0 \; and x > a)$

Or $\quad\quad |A|^2 \int_0^a \sin^2 \frac{n\pi x}{a} dx = 1$

Or $\quad\quad |A|^2 \int_0^a \frac{(1 - \cos 2n\pi x)}{2} dx = 1 \quad \text{.....................} \quad \text{L7.12}$

$$\frac{|A|^2}{2} \left[x - \frac{\sin \frac{2n\pi x}{a}}{\frac{2n\pi}{a}} \right]_0^a = 1$$

Or $\quad\quad \frac{|A|^2}{2} \left[(a - 0) - \frac{a}{2n\pi} (\sin 2n\pi - \sin 0) \right] = 1$

Or $\quad\quad \frac{|A|^2}{2} [(a - 0)] = 1$

Or $\quad\quad \frac{|A|^2}{2} a = 1 \quad$ or $|A|^2 = \frac{2}{a}$

$$A = \sqrt{\frac{2}{a}} \quad \text{...} \quad \text{L7.13}$$

So, $\quad \boldsymbol{\Psi_n(x)} = \sqrt{\frac{2}{a}} \boldsymbol{\sin} \frac{n\pi x}{a} \quad \text{...................................} \quad \text{L7.14}$

Eqn. (L7.14) gives the normalized eigen function of the particle enclosed in infinitely deep potential well. Substituting n=1,2,,3,............, in eqn. (L7.14) we get

$$\Psi_1(x) = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}$$

$$\Psi_2(x) = \sqrt{\frac{2}{a}} \sin\frac{2\pi x}{a}$$

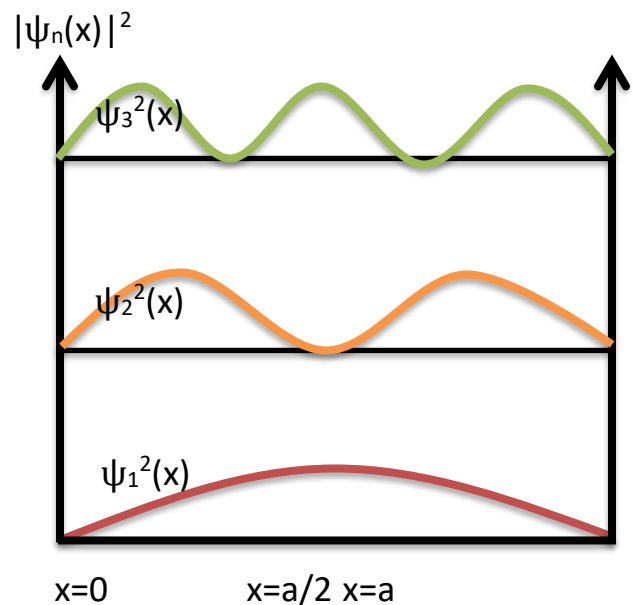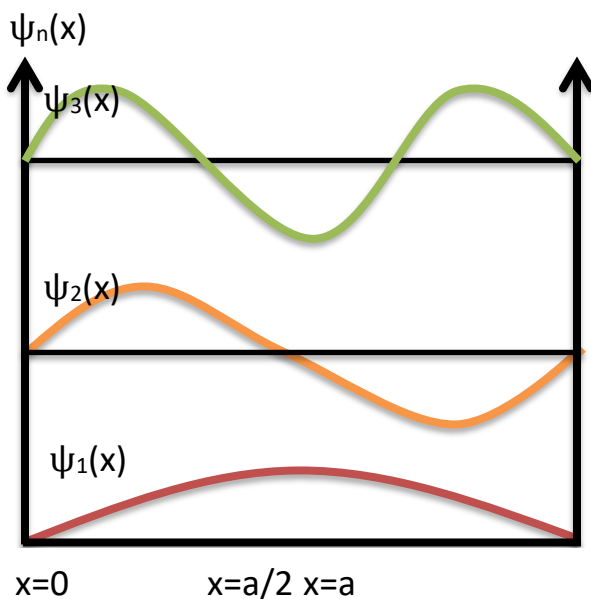$\Psi_3(x) = \sqrt{\frac{2}{a}} \sin\frac{3\pi x}{a}$etc.

Now the probabilities of finding the particle inside the potential well is given by

$$|\Psi_n(x)|^2 = \frac{2}{a}\sin^2\frac{n\pi x}{a} \qquad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(L7.15)$$

Substituting n=1,2, 3…….. the corresponding probability of finding the particle in eigen states Ψ_1, Ψ_2, Ψ_3 are given by

$$|\Psi_1(x)|^2 = \frac{2}{a}\sin^2\frac{\pi x}{a}$$

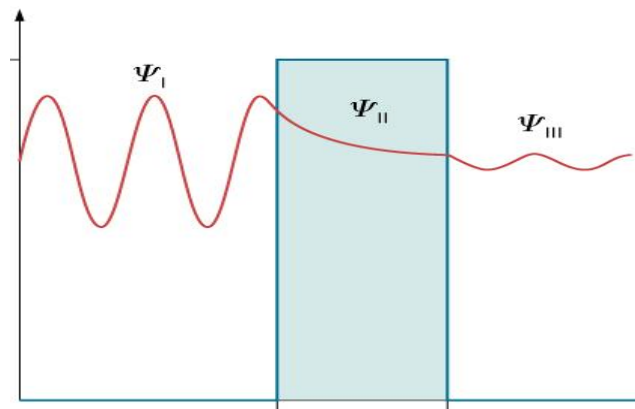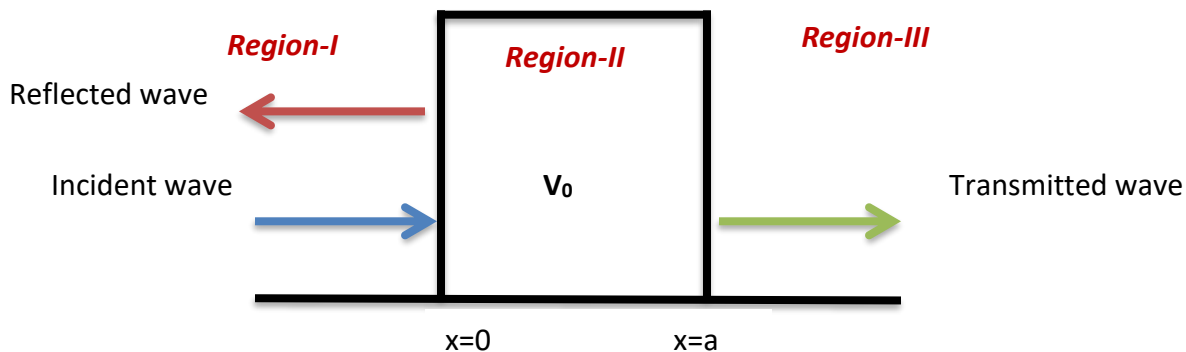$$|\Psi_2(x)|^2 = \frac{2}{a}\sin^2\frac{2\pi x}{a}$$

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Lecture-8

Square well potential barrier and Quantum mechanical tunneling (concepts)

The square potential barrier function can be written as

$$V(x) = \begin{cases} 0 \text{ for } x<0 \\ V_0 \text{ for } 0<x<a \\ 0 \text{ for } x>a \end{cases} \quad \text{.............................} \quad L8.1$$

Region-I

Region-II

Region-III

Reflected wave

Incident wave

V_0

Transmitted wave

x=0   x=a

Ψ_I

Ψ_{II}

Ψ_{III}

Consider a stream of particles of mass m approaching the square barrier from left. Classically, if the particle energy is less than the barrier height ($E<V_0$), it's always reflected where as its transmitted if $E>V_0$. However, quantum mechanically it can be seen that there is always a finite probability for a particle to penetrate or leak through the barrier and continue its forward motion even if $E<V_0$. This phenomenon is known as *Quantum mechanical tunneling*.

Module 3
Elementary Quantum Mechanics & Application of Quantum Mechanics
Quantum confinements and Applications of Nanoscience in Quantum mechanics:

Quantum confinement refers to the effect that occurs when the motion of electrons is restricted in one or more dimensions, leading to the discretization of energy levels. This phenomenon is commonly observed in semiconductor nanostructures, where it causes changes in the electronic, optical, and transport properties of materials. In quantum confinement, electrons exist in potential wells, resulting in distinct energy levels and band gaps that differ from those in bulk materials.

Quantum Dots: Nanocrystals that exhibit size-dependent optical properties, making them useful for applications in display technologies, biological imaging, and solar cells. For example, quantum dots can be engineered to emit specific colors of light based on their size, improving color purity in displays.

Light-Emitting Diodes (LEDs): Quantum wells are utilized in semiconductor lasers and LEDs to enhance light emission efficiency and allow for tunable wavelengths

Drug Delivery: Quantum dots can be used as carriers for targeted drug delivery due to their surface modification capabilities and ability to be tracked in vivo using fluorescence.

Nanocomposites: Quantum confined materials can be incorporated into polymer matrices to improve mechanical, thermal, or electrical properties, resulting in advanced materials for various industrial applications.