

## **UNIT-I: syllabus**

Quantum Mechanics Introduction to quantum physics, Black body radiation, Planck's law, Photoelectric effect, Compton effect, de-Broglie's hypothesis, Wave-particle duality, Davisson and Germer experiment, Heisenberg's Uncertainty principle, Born's interpretation of the wave function, Schrodinger's time independent wave equation, Particle in one dimensional box.

### **UNIT- I**

## **QUANTUM MECHANICS**

Quantum Mechanics: - It is the branch of Physics, which explains the motion of microscopic particles like electrons, protons.. etc. It is introduced by Max Planck in 1900, developed by Einstein.

Classical Mechanics: - It is the branch of Physics, which explains the motion of macroscopic objects. It is introduced by Issac Newton in 1684.

### Blackbody radiation

A blackbody is a body which absorbs radiation of all wavelengths incident upon it. It neither reflects nor transmits any of the incident radiation and therefore appears black irrespective of the colour of the incident radiation. When a blackbody is heated it emits radiation known as blackbody radiation.

A blackbody devised by Ferry consists of a hollow thick-walled sphere painted lamp black internally provided with a small circular opening for the radiation to enter. There is a projection to prevent direct reflection in front of the opening. When any radiation enters the opening suffers multiple reflections inside the sphere and is finally absorbed.

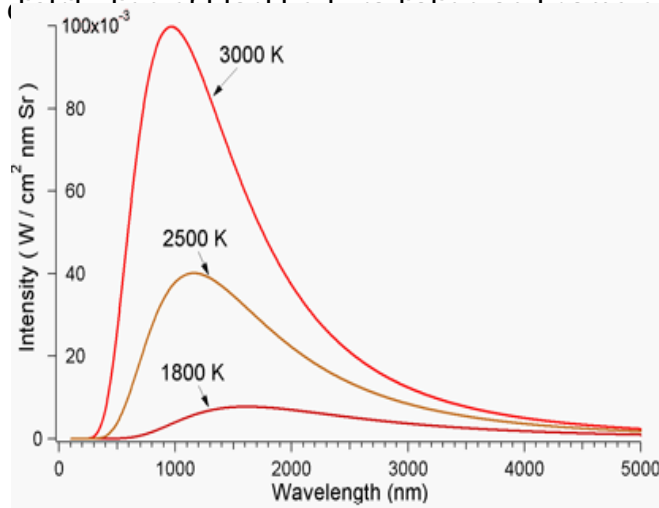
When the walls of such cavity are heated to a temperature  $T$ , the radiation emitted fills the cavity and leaves from the opening. The emitted radiation is called as Blackbody radiation which is a characteristic of the temperature of the body and is independent of the type of the material.

### Spectral Distribution

Stefan-Boltzmann in 1884 showed that the radiation energy per unit volume due to all wavelengths is proportional to the fourth power of absolute temperature of the blackbody known as Stefan's fourth power law.

### Lummer and Pringsheim's Experimental Findings

Lummer and Pringsheim have carried out various experiments on the spectral distribution of blackbody radiation. The following graph shows the results of their experiments with the important findings as follows.



The energy is not uniformly distributed in the radiation spectrum of a blackbody as shown in fig 1.1.

For a given temperature, the intensity of the radiation increases with increase in wavelength and becomes maximum for a particular wavelength.

With further increase in the wavelength, the intensity of radiation decreases.

The wavelength corresponding to the maximum intensity represented by the peak of the curve shifts towards shorter wavelengths as the temperature increases.

### Wien's Law

In order to explain the observed spectral distribution, Wein in 1893 showed that the energy density in

the wavelength range  $\lambda$  and  $\lambda+d\lambda$  is given by  $E_{\lambda}d\lambda = K\lambda^{-5} e^{\left(\frac{-a}{\lambda T}\right)}d\lambda$ , where  $a$  &  $K$  are constants,  $T$  is the absolute temperature of the blackbody. Wien's formula works out for

shorter wavelengths, but has considerable deviations for long wavelengths and high temperatures.

### Rayleigh-Jeans Formula

In 1900, Rayleigh and Jeans used a more vigorous method and obtained the following formula for the energy distribution as,  $E_\lambda d\lambda = B\lambda^{-4} T e^{\left(\frac{-a}{\lambda T}\right)} d\lambda$ , where  $B$  is a constant.

It can be rewritten in the form,  $E_\lambda d\lambda = 8\pi kT \lambda^{-4} d\lambda$ .

It was found that Rayleigh-Jeans formula is in coincidence with the experimental results only in the longer wavelength region.

### Planck's Law

In 1900, Max Planck suggested that the correct results on the spectral distribution of blackbody radiation can be obtained by considering the energy of the oscillating particles to be discrete rather than continuous. He derived the radiation law using the following assumptions.

A chamber containing blackbody radiations also contains simple harmonic oscillators of molecular dimensions which can vibrate with all possible frequencies.

The frequency of radiation emitted by an oscillator is the same as the frequency of its vibration.

An oscillator cannot emit energy in a continuous manner, it can emit energy in the multiples of a small unit called quantum. If an oscillator is vibrating with a frequency ' $\nu$ ', it can only radiate in quanta of magnitude  $h\nu$ , i.e., the oscillator can have only discrete values of energy given by  $E_n = nh\nu = n\varepsilon$ , where  $h\nu = \varepsilon$ ,  $n$  is an integer and  $h$  is Planck's constant =  $6.625 \times 10^{-34}$ .

The oscillator can emit or absorb radiation energy in packets of  $h\nu$ . This implies that the exchange of energy between radiation and matter cannot take place continuously but are limited to discrete set of values  $0, h\nu, 2h\nu, 3h\nu, \dots, nh\nu$ . →[1]

Let there be  $N_0, N_1, N_2, \dots, N_r, \dots$  etc. oscillators having energy  $0, \varepsilon, 2\varepsilon, 3\varepsilon, \dots, r\varepsilon, \dots$  etc. respectively. Now we have  $N = N_0 + N_1 + N_2 + \dots + N_r + \dots$

→[2]

And  $E = 0 + \varepsilon N_1 + 2\varepsilon N_2 + 3\varepsilon N_3 + \dots + r\varepsilon N_r + \dots$   
→[3]

If  $N$  is the no. of Planck's oscillators and  $E$  be their total energy, then the average energy per

Planck's oscillator of energy  $E$  is given by  $\bar{\varepsilon} = \frac{E}{N}$

According to Maxwell's distribution formula, the no. of oscillators having energy  $r\varepsilon$  is given by,

$$N_r = N_o e^{\left(\frac{-r\varepsilon}{kT}\right)}, \text{ where } k \text{ is Boltzmann's constant.}$$

→[4]

$$\text{Total number of oscillators} = N = \frac{N_o}{\{1 - e^{\left(\frac{-\varepsilon}{kT}\right)}\}} \left( \because 1 + x + x^2 + x^3 + \dots = \frac{1}{1-x} \right) \rightarrow [5]$$

The total energy  $E$  is given by

$$\begin{aligned} E &= (N_o \times 0) + \varepsilon N_o e^{\left(\frac{-\varepsilon}{kT}\right)} + 2\varepsilon N_o e^{\left(\frac{-2\varepsilon}{kT}\right)} + 3\varepsilon N_o e^{\left(\frac{-3\varepsilon}{kT}\right)} \dots + r\varepsilon N_o e^{\left(\frac{-r\varepsilon}{kT}\right)} + \dots \\ &= \varepsilon N_o e^{\left(\frac{-\varepsilon}{kT}\right)} \left[ 1 + 2e^{\left(\frac{-\varepsilon}{kT}\right)} + 3e^{\left(\frac{-2\varepsilon}{kT}\right)} \dots + re^{\left(\frac{-(r-1)\varepsilon}{kT}\right)} + \dots \right] \rightarrow [6] \\ &= \left[ \frac{\varepsilon N_o e^{\left(\frac{-\varepsilon}{kT}\right)}}{\{1 - e^{\left(\frac{-\varepsilon}{kT}\right)}\}^2} \right] \quad \left[ \because 1 + 2x + 3x^2 + \dots + rx^{r-1} = \frac{1}{(1-x^2)} \right] \end{aligned}$$

→[7] Now the average energy of the oscillator is given by,

$$\bar{\varepsilon} = \frac{E}{N} = \frac{\varepsilon N_o \exp(-\varepsilon / kT) / \{1 - \exp(-\varepsilon / kT)\}^2}{N_o / \{1 - \exp(-\varepsilon / kT)\}} = \frac{\varepsilon \exp(-\varepsilon / kT)}{\{1 - \exp(-\varepsilon / kT)\}} = \frac{\varepsilon}{\{\exp\left(\frac{\varepsilon}{kT}\right) - 1\}} = \frac{h\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1}$$

→[8]

The no. of oscillators per unit volume in the range between  $\nu$  and  $\nu + d\nu$  is given

$$\text{as, } N = \frac{8\pi\nu^2}{C^3} d\nu \rightarrow [9]$$

The radiation energy density, i.e. the energy per unit volume within the interval  $d\nu$  is given as the product of no. of oscillators per unit volume in the same interval and the average energy of oscillator.

$$\text{i.e., } E_\nu d\nu = \frac{8\pi\nu^2}{C^3} d\nu \times \frac{h\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1} \Rightarrow E_\nu d\nu = \frac{8\pi h\nu^3}{C^3} \frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1} d\nu$$

→[10]

Equation [10] is known as Planck's radiation law.

It is also expressed in terms of wavelength as  $E_\lambda d\lambda = \frac{8\pi hC}{\lambda^5} \frac{1}{\exp\left(\frac{hC}{\lambda kT}\right) - 1} d\lambda$

→[11]

This formula agrees well with the experimental curves throughout the whole range of wavelengths.

### Photoelectric Effect

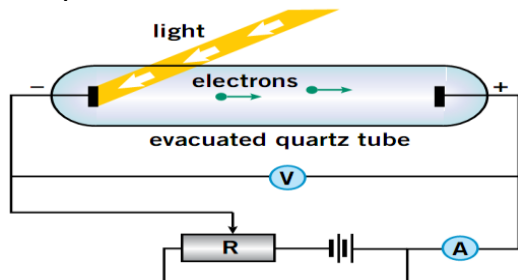
The emission of electrons from a metal plate when illuminated by light or any other radiation of suitable wavelength (or frequency) (ultraviolet light on zinc plate and ordinary light on alkali metals such as sodium, potassium, lithium) is called photoelectric effect. The emitted electrons are called as photoelectrons and the phenomenon is called as photoelectric effect.

### Experimental study of photoelectric effect

A simple experimental arrangement to study the photoelectric effect is shown in fig 1.2. The apparatus consists of two photosensitive surfaces A and B, enclosed in an evacuated quartz bulb. The plate A is connected to the negative terminal of a potential divider while the plate B is connected to the positive terminal through a galvanometer G or micro ammeter. In the absence of any light there is no flow of current and hence there is no deflection in the galvanometer or micro-ammeter. But when monochromatic light is allowed to fall on plate A, current starts flowing in the circuit which is indicated by

galvanometer. The current is known as photocurrent. This shows that when the light falls on the metallic surface, electrons are ejected. The number of electrons emitted and their kinetic energy depends up on the following factors

The potential difference between the two electrodes



i.e. between plates A and B

The intensity of incident radiation

The frequency of incident radiation

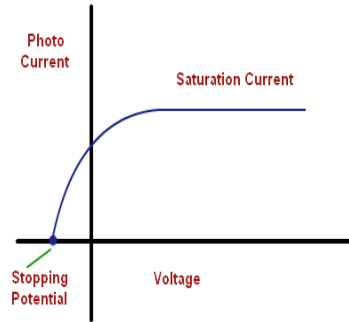
The photo metal used

Characteristics of photo electrons

The effect of potential difference

For a given photo metallic surface A, keeping the intensity and frequency of incident radiation fixed, let us consider the effect of potential difference between the plates.

Figure 4.2.4 Variation of photoelectric current (no. of emitted photoelectrons)



as a function of potential difference  $V$  between the two plates

. When the positive potential of the plate  $B$  is increased, photoelectric current is also increased and reaches a certain maximum value.

This value of the current is known as saturation current.

Further increase in the potential hardly produces any appreciable increase in current. If the potential difference is kept zero,

it is observed that photoelectric current still flows in the same direction.

This shows that the incident radiation not only provides a conducting path

but in addition an electromagnetic force to photoelectrons.

If the potential of the plate  $B$  is made negative, the photocurrent does not immediately drop to zero but flows in the same direction as for positive potentials. This shows that the photoelectrons are emitted from the plate  $A$  with a finite velocity. If the negative or retarding potential is further increased, the photocurrent decreases and finally becomes zero at a particular value. The negative potential of the plate  $B$  at which the photoelectric current becomes zero is called as cut off potential or stopping potential. Thus stopping potential is that value of retarding potential difference between two electrodes which is just sufficient to haul the most energetic photoelectrons emitted.



## Effect of intensity of incident radiation

Let us consider the effect of intensity of incident radiation course of the same frequency.

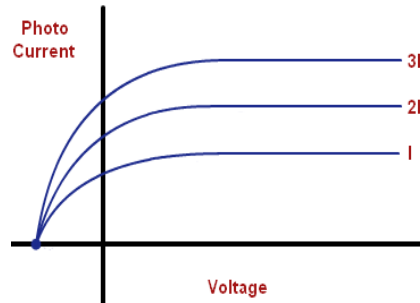


Fig 1.3.2 shows the variation of photocurrent as a function of potential difference between the two plates for different intensities of incident radiation.

If the intensity of incident radiation is increased from  $I$  to  $2I$  and the experiment is repeated then the photoelectric current increases in the same ratio for all positive values of  $V$ .

As  $V$  is made negative, the photoelectric current decreases sharply and reaches zero at same value of the voltage  $V_0$ , called as the stopping potential.

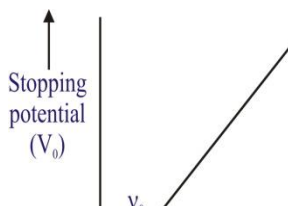
Hence we conclude that

the stopping potential is independent of intensity of incident radiation

the saturation current is proportional to the intensity of incident radiation

i.e. higher the intensity of radiation higher the saturation current.

Now we shall consider the effect of varying frequency of the incident radiation while keeping the same emitting surface and same intensity of incident radiation.



. Fig.1.3.3 shows the variation of stopping potential with frequency

Fig.1.3.3 shows the variation of stopping potential with frequency of incident light. Here stopping potentials are measured for different frequencies. The graph shows that at frequency  $\nu_0$ , the stopping potential is zero. The frequency  $\nu_0$  is known as threshold frequency and the wavelength corresponding to threshold frequency is called as threshold wavelength.

The photoelectric effect occurs above this frequency while ceases below this frequency. Hence the threshold frequency is defined as the minimum frequency ( $\nu_0$ ) of the incident radiation which can cause photoelectric emission i.e. this frequency is just able to liberate electrons without giving them additional energy.

Effect of photo metal

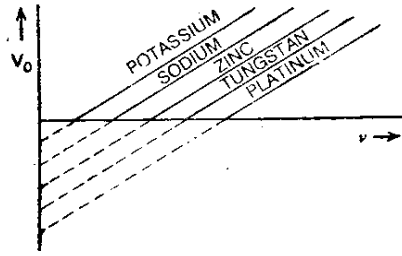


Fig. 1.3.4 shows graph between stopping potential  $V_0$  and frequency for a number of photo-metals. It is clear from the graph that all the lines have the same slope but their intersections with frequency axis are different. Thus we conclude the threshold frequency is function of the photo-metal i.e. it depends on the nature of the photo-metal.

### Fundamental laws of photoelectric emission

Following are the fundamental laws of photoelectric emission.

The number of electrons emitted per second i.e., photoelectric current is proportional to the intensity of incident light.

For a given material, there exists a certain minimum frequency of the incident light so that photoelectrons can be ejected from metal surface. If the frequency is less than this frequency no electrons can be emitted from the metal surface however intense incident light may be. The minimum value of the frequency is known as threshold frequency and the corresponding wavelength as threshold wavelength.

The maximum velocity or the kinetic energy of photo electron depends on the frequency of radiation and not on intensity. The kinetic energy of photoelectrons increases with increase in frequency of incident light.

The rate at which the electrons are emitted from a photo cathode is independent of its temperature. This shows that photoelectric phenomenon is entirely different from thermionic emission.

Electron emission from the photosensitive surface is almost instantaneous and emission continues as long as frequency of incident radiation is greater than the threshold frequency. The time lag between the incidence of radiation and the emission of electrons is less than  $10^{-8}$  seconds.

For a given metal surface, stopping potential  $V_0$  is directly proportional to frequency but is independent of the intensity of incident light.

### Einstein's Photo-electric Equation

Following Planck's idea that light consists of photons Einstein proposed an explanation of photoelectric effect as early as 1905. According to this, in photoelectric effect one photon is completely absorbed by one electron, which thereby gains the quantum of energy and may be emitted from the metal. The photon's energy is used in the following two parts.

A part of its energy is used to free electron from the atom and away from the metal surface. This energy is known as photoelectric work function of the metal. This is denoted by  $W_0$ .

The other part is used in giving kinetic energy ( $\frac{1}{2}mv^2$ ) to the electron. Thus

$$h\nu = W_0 + \frac{1}{2}mv^2 \quad \rightarrow [1]$$

Where  $v$  is the velocity of the emitted electron, equation [1] is known as Einstein's photoelectric equation.

When the photon's energy is of such a value that it can only liberate the electron from metal, then the kinetic energy of the electron will be zero. Equation [1] now reduces to,  $h\nu_0 = W_0$ , where  $\nu_0$  is called as threshold frequency, which is defined as the minimum frequency which can cause photoelectric emission. If the frequency of the incident photon is below threshold frequency no emission of electrons will take place.

Corresponding to threshold frequency we define long wavelength limit  $\lambda_0$ . It represents an upper limit of wavelength for photoelectric effect. Its physical significance is that radiations having wavelength longer than  $\lambda_0$  would not be able to eject electrons from a given metal surface, whereas those having  $\lambda < \lambda_0$  will. The value of  $\lambda_0$  is given by  $c = \nu_0 \lambda_0$ . As

$$W_0 = h\nu_0 = \frac{hc}{\lambda_0} \Rightarrow \lambda_0 = \frac{hc}{W_0 \text{ (in J)}} \text{ (m)} = \frac{12400}{W_0 \text{ (in eV)}} \text{ \AA} \quad \rightarrow [2]$$

From equation [1], we can write,  $\frac{1}{2}mv^2 = h\nu_o - W_o$ . Since work function for a material is constant,

$$v^2 \propto \nu.$$

Thus the increase in frequency  $\nu$  of incident light causes increase in velocity of photoelectrons provided intensity of incident light is constant. An increase in the intensity of radiation is equivalent to an increase in the number of photons falling on the emitting surface. If the frequency of incident radiation is above the threshold frequency ( $\nu > \nu_o$ ), then the number of emitted electrons will increase. In this way the intensity of emitted electrons is directly proportional to the intensity of incident radiation.

### Compton Effect

In 1921, Prof. A.H. Compton discovered that when a monochromatic beam of high frequency radiation (x-rays,  $\gamma$ - rays) is scattered by a substance, the scattered radiation consists of two components,

One having the same frequency or same wavelength called as unmodified radiation  
the other having lower frequency or higher wavelength called as modified radiation.

Compton explained this phenomenon on the basis of Quantum theory of radiation. According to Quantum theory of radiation, radiation is constituted of energy packets called photons whose energy is  $h\nu$  which move with a velocity  $C$  and have momentum ( $h\nu/C$ ). They obey the laws of conservation energy and momentum when they are scattered by a substance.

According to Compton, the phenomenon of scattering is due to an elastic collision between the photon of the radiation and the electron of the scatterer.

As the photon collides with an electron it transfers some energy to it and gets scattered in a different direction with reduced energy, thus a lowered frequency. The electron recoils in another direction due to this gain in energy. The observed change in frequency or wavelength of the scattered radiation is called as Compton's shift and the phenomenon is known as Compton Effect.

## Expression for Compton shift

Let a photon of energy  $h\nu$  collides with an electron at rest as shown in fig 1.4. During this collision a fraction of energy is transferred to the electron which gains kinetic energy and recoils. This collision produces scattering photon and recoiling electron in different

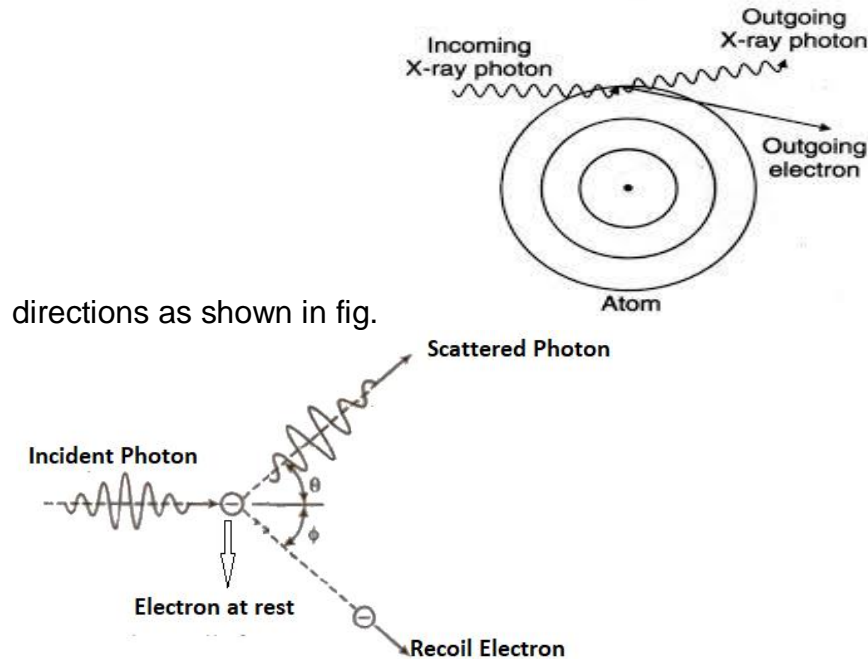


Fig 1.4

Before collision:

Energy of incident photon  $= h\nu$

Momentum of incident photon  $= \frac{h\nu}{C}$

Rest energy of electron  $= m_0 C^2$

Momentum of the electron  $= 0$

After collision:

Energy of the scattered photon  $= h\nu'$

Momentum of the scattered photon  $= \frac{h\nu'}{C}$

Energy of electron

$=mC^2$  ( $m$ =relativistic mass of electron, given as

$$m = \frac{m_o}{\sqrt{1 - \frac{v^2}{C^2}}}$$

Momentum of the recoil electron  $= mv$

Using the law of conservation of energy:

$$\text{We have } h\nu + m_o C^2 = h\nu' + mC^2$$

$\rightarrow [1]$

Using the law of conservation of momentum:

$$\text{in the direction of incident photon, we get, } \frac{h\nu}{C} + 0 = \frac{h\nu'}{C} \cos \theta + mv \cos \phi \quad \rightarrow [2]$$

in the direction perpendicular to the direction of incident photon, we get,

$$0 + 0 = \frac{h\nu'}{C} \sin \theta - mv \sin \phi \quad \rightarrow [3]$$

From [2],

$$mvC \cos \phi = h\nu - h\nu' \cos \theta \quad \rightarrow [4]$$

& from [3],

$$mvC \sin \phi = h\nu' \sin \theta \quad \rightarrow [5]$$

Squaring and adding [4] and [5], we get

$$m^2 v^2 C^2 = h^2 [\nu^2 + \nu'^2 - 2\nu\nu' \cos \theta]$$

$\rightarrow [6]$

From equation [1], we have

$$mC^2 = h(\nu - \nu') + m_o C^2$$

$\rightarrow [7]$

On squaring [7],

$$m^2 C^4 = [h(\nu - \nu') + m_o C^2]^2$$

$$\text{i.e. } m^2 C^4 = h^2 (\nu - \nu')^2 + 2h(\nu - \nu') m_o C^2 + m_o^2 C^4$$

$\rightarrow [8]$

Taking [7]-[6], substituting  $m = \frac{m_o}{\sqrt{1 - \frac{v^2}{C^2}}}$  and reducing, we get to  $\frac{1}{v'} - \frac{1}{v} = \frac{h}{m_o C^2} (1 - \cos \theta)$

→[9]

Which shows that  $v' < v$ . Multiplying [9] with C,

$$\lambda - \lambda' = \Delta\lambda = \frac{h}{m_o C} (1 - \cos \theta) = \frac{2h}{m_o C} \sin^2 \left( \frac{\theta}{2} \right) \rightarrow [10]$$

we get,

Equation [10] is a mathematical expression for the Compton Shift.

## Dual Nature of Radiation

To understand the concept of dual nature of radiation we should understand what a particle is and what a wave is. The particle can be specified by parameters like its mass, velocity, momentum and energy. A wave is nothing but a spread out disturbance which is specified by parameters like its frequency, wavelength, phase, amplitude and intensity.

Radiation including visible light, infrared, ultraviolet, X-rays etc. behaves as a -wave in experiments based on interference, diffraction etc. This is due to the fact that these phenomena require the presence of two waves at the same position at the same time. However, it is difficult for two particles to occupy the same position at the same time. Thus we conclude that radiation behaves like wave.

Planck's quantum theory was successful in explaining black body radiation, the photoelectric effect, the Compton Effect etc. and had clearly established that radiation in its interaction with matter behaves as if it consists of particles. Here radiation interacts with matter in form of quanta or photon. Thus we conclude that radiation behaves like particle.

Radiation sometimes behaves like a wave and sometimes behaves like a particle which is referred to as wave-particle dualism. However radiation cannot exhibit both particle and wave natures simultaneously.

## de Broglie Concept

Louis de-Broglie in 1924 extended the wave-particle parallelism of radiation to all fundamental material particles like electrons, protons, neutrons, atoms and molecules,



stating that “every material particle in motion is associated with a wave, whose wavelength is inversely proportional to its momentum”. The corresponding wavelength is called as de-Broglie wavelength which is given as,  $\lambda = \frac{h}{mv}$ , where  $h$  is Planck’s constant,  $m$  and  $v$  are the mass and velocity

### Waves & Particles:-

Wave:- A wave is nothing but spreading of disturbance created in a medium. The characteristics of waves are

1) amplitude 2) time period 3) frequency 4) wave length 5) phase  
6) intensity

Particle:- It is a smallest quantity of substance of matter which occupies a certain space, is called as a particle.

The characteristics of a particle are 1) Mass 2) velocity 3) momentum 4) energy

Matter waves:- *The waves associated with a material particles are called as matter waves.*

### de- Broglie concept of Dual nature of Matter waves :-

The universe is made up of radiation (light) and matter (particles). The light exhibits dual nature.

They are , 1. Wave nature                      2. Particle nature

Wave nature of light is verified by interference, diffraction and polarization phenomenon etc.

Particle nature of light is verified by Photo electric effect, Compton effect etc .

In 1924 Louis de-Broglie suggested that , matter waves also exhibit dual nature like radiation (light) .

They are , 1. Wave nature                      2. Particle nature

Wave nature of matter waves is verified by Davisson & Germer’s experiment, G.P. Thomson experiment etc.

Particle nature of matter wave is verified by Geiger –Muller counter, Wilson cloud chamber, Bubble chamber etc.

### de-Broglie Hypothesis:-

In 1924, de-Broglie made few hypothesis for dual nature of matter waves. They are

1. The universe consists of matter and radiation (light) only
2. Nature loves symmetry
3. Matter waves also exhibits dual nature like radiation
4. The waves associated with material particles are called as matter waves or de-Broglie matter

waves & its wavelength is called as de-Broglie wave length.

5. de-Broglie wave length,  $\lambda = \frac{h}{p} = \frac{h}{mv}$

### de-Broglie wavelength ( $\lambda$ ) expression:-

According to the Planck's theory of radiation, the energy of a photon is given by

$E = hv = hc/\lambda$  .....(1), where  $h$  = Planck's constant,  $v$  = frequency of a photon

According to Einstein's Mass- Energy relation,

$E = mc^2$ .....(2) , where  $m$  = mass of a photon,  $c$  = velocity of a photon

From equations (1) and (2),  $hc/\lambda = mc^2$

$$h = \lambda mc \Rightarrow \lambda = h/mc$$

$$= h/mv \quad [\text{since, } v = c]$$

But according to de-Broglie, momentum  $P = mv$ ,

Therefore,  $\lambda = \frac{h}{p} = \frac{h}{mv}$  ..... (3)

Case (i) de-Broglie Wavelength in terms of Energy (E):-

We know that the kinetic energy,  $E = \frac{1}{2} mv^2$

Multiply by 'm' on both sides, we get

$$m.E = \frac{1}{2} m^2 v^2 \quad \Rightarrow \quad 2 m .E = m^2 v^2 \quad \text{and} \quad mv = \sqrt{2mE}$$

But, de-Broglie wave length  $\lambda = \frac{h}{mv} \Rightarrow \lambda = \frac{h}{\sqrt{2mE}} \dots\dots\dots (4)$

Case (ii) de-Broglie Wavelength in terms of Voltage (V):-

If a charged particle of charge 'e' is accelerated through a potential difference of 'V' volts, then the kinetic energy of the particle is ,  $E = eV \dots\dots (5)$

But, de-Broglie wavelength,  $\lambda = \frac{h}{\sqrt{2mE}} \Rightarrow \boxed{\lambda = \frac{h}{\sqrt{2meV}} = \frac{12.27}{\sqrt{V}} \text{ \AA}}$

Where, h = Planck's constant =  $6.63 \times 10^{-34}$  j-s, m = mass of electron =  $9.1 \times 10^{-31}$  kg,

$E =$  charge of electron =  $1.6 \times 10^{-19}$ c,  $1\text{ev} = 1.6 \times 10^{-19}$  j,  $1\text{\AA} = 10^{-8}$  cm.

Case (iii) de-Broglie wavelength in terms of Temperature (T):-

According to the kinetic theory of gases, the average kinetic energy of a particle at temperature 'T' is given by,

$E = \frac{3}{2} K_B T$  , where  $K_B T$  is Boltz mann constant.

But, de-Broglie wave length  $\lambda = \frac{h}{\sqrt{2mE}}$

$$\Rightarrow \boxed{\lambda = \frac{h}{\sqrt{3mK_B T}}}$$

Properties (or) Characteristics of Matter waves:-

The de-Broglie wavelength,  $\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2meV}} = \frac{h}{\sqrt{3mK_B T}}$

1. The lighter the particle, greater is the wavelength associated with it.
2. Lesser the velocity of the particle, longer the wavelength associated with it .
3. When  $v = 0$  then  $\lambda = \infty$  and  $v = \infty$  then,  $\lambda = 0$

The experimental set up is shown in fig.1. It consists of mainly 3 parts.

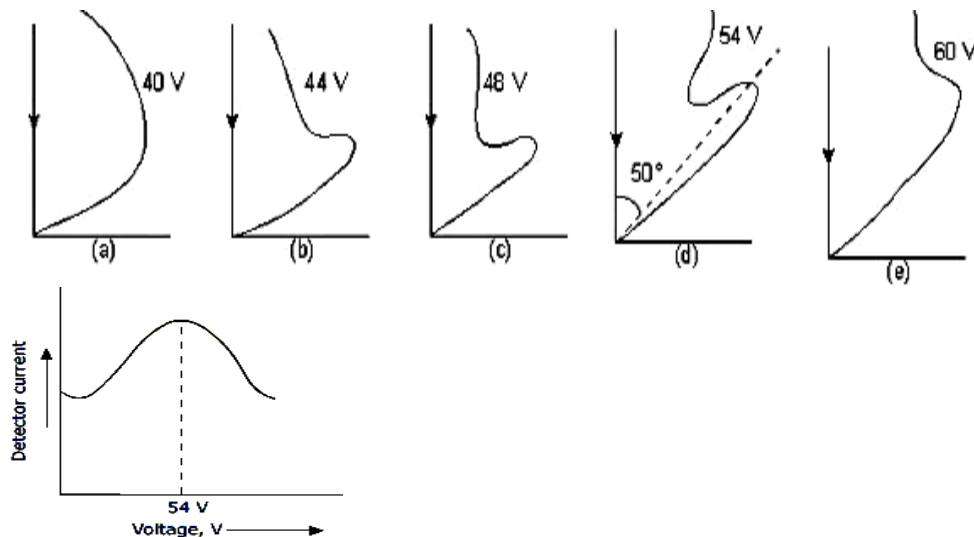
(i) Filament (ii) Target (iii) Circular Scale arrangement.

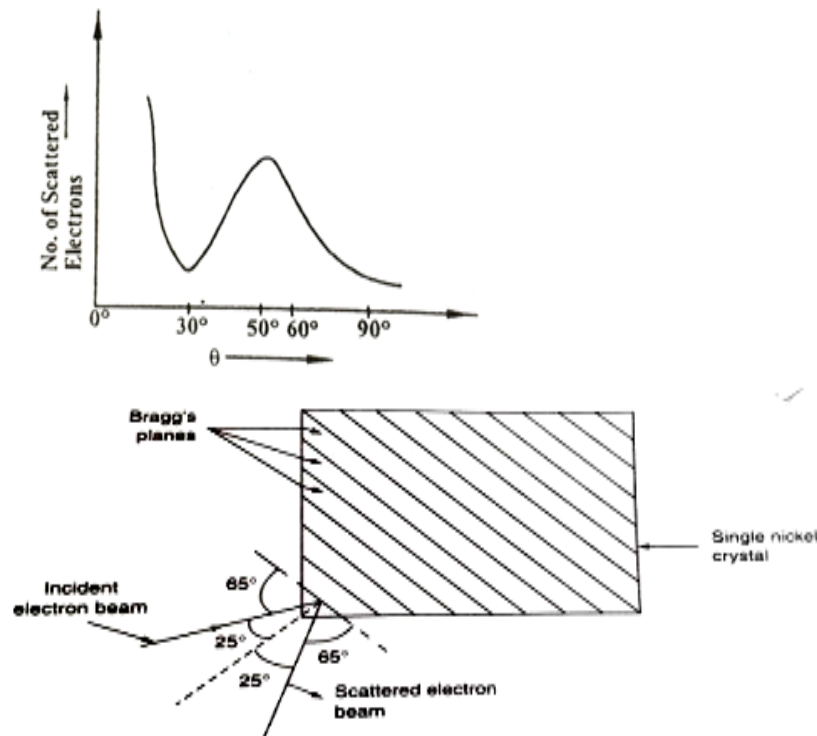
It also consists of a low tension battery (LTB), High tension battery (HTB) & a cylinder.

When tungsten filament 'F' is heated by a LTB then electrons are produced. These electrons are accelerated by applying high tension battery (HTB). These accelerated electrons are collimated into a fine beam of pencil by passing them through a system of pin holes in the cylinder 'A'.

This beam of electrons is allowed to incident on *Nickel crystal* which acts as target. Then electrons are scattered in all directions. The intensity of scattered electrons is measured by the circular scale arrangement. In this arrangement, an electron collector is fixed to a circular scale which can collect the electrons and can move along the circular scale. The electron collector is connected to a sensitive galvanometer to measure the intensity of electron beam entering the collector at different scattering angles.

Graphs:-





The electron beam is accelerated by 54 Volts is made to strike the Nickel crystal and a sharp maximum is occurred at scattering angle  $\phi = 50^\circ$  of the incident beam. The incident beam and the diffracted beam in this experiment make an angle of  $\theta = 65^\circ$  with the family of Bragg's planes.

Theoretical ' $\lambda$ ' value:-

$d = 0.091\text{nm}$  (for Nickel crystals)

According to Bragg's law for maxima in diffracted pattern,  $2d \sin \theta = n\lambda$

For  $n = 1$ ,  $\lambda = 2d \sin \theta$

$$= 2 \times 0.91 \times 10^{-10} \times \sin 65^\circ = 0.165 \text{ nm}$$

$$\lambda = 1.65 \text{ \AA} \dots\dots\dots(1)$$

Experimental ' $\lambda$ ' value:-

For a 54 V electron, the deBroglie wavelength associated with the electron is given by

$$\lambda = 12.25 / \sqrt{V} = (12.27 / \sqrt{54})\text{\AA} = 1.66 \text{ \AA} \dots\dots\dots(2)$$

Equation (1) is matched with equation (2). This confirms the existence of matter waves.

i.e, the wave nature of matter (particle or electrons) is verified experimentally.

Drawback:- It fails to explain the diffraction pattern whether it is formed due to electrons (or) Electromagnetic radiation generated by fast moving electrons.

### HEISENBERG UNCERTAINTY PRINCIPLE:-

From the de-Broglie hypothesis we can confirm that the electron can behave both as a particle and as a wave. This dual behaviour of electron makes difficult in locating the exact position and momentum of the electrons, simultaneously. This is called uncertainty. This difficulty is solved by Heisenberg in 1927, with the principle called as Heisenberg uncertainty principle.

#### Statement:-

“It is impossible to measure both the position and momentum of a particle simultaneously to any desired degree of accuracy”.

If  $\Delta X$  is the uncertainty (error) in determining the position and  $\Delta P$  is the uncertainty (error) in determining the momentum, then these uncertainties can be related as,  $\Delta X \cdot \Delta P \geq \frac{h}{4\pi}$

Heisenberg Uncertainty principle, in other forms:- i.  $\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$

$$\text{ii. } \Delta J \cdot \Delta \theta \geq \frac{h}{4\pi}$$

#### Applications:-

1. It explains the non-existence of electrons in the nucleus.
2. It explains the existence of protons & neutrons in the nucleus.
3. It gives the binding energy of an electron in atom.
4. It calculates the radius of Bohr's first orbit.

### SCHRODINGER WAVE EQUATION:-

Schrodinger described the wave nature of a particle in mathematical form and is known as Schrodinger wave equation. These are of two types:

1). Time independent wave equation.  $[\nabla^2 \Psi + [2m(E - V)/\hbar^2] \Psi = 0]$

2). Time dependent wave equation.  $[E^{\wedge} \Psi = H^{\wedge} \Psi]$  (or)

$$(i\hbar \frac{\partial}{\partial t}) \Psi = (-\frac{\hbar^2}{2m} \nabla^2 + V) \Psi$$

Where,  $H^{\wedge}$  = Hamilton operator,  $E^{\wedge}$  = Energy operator

### 1.SCHRODINGER TIME INDEPENDENT WAVE EQUATION:-

Schrödinger, in 1926, developed wave equation for the moving particles. One of its forms can be derived by simply incorporating the deBroglie wavelength expression into the classical wave equation.

If a particle of mass 'm' moving with velocity 'v' is associated with a group of waves. Let  $\psi$  be the wave function of the particle. Also let us consider a simple form of progressing wave like the one represented by the following equation,

$\Psi = \Psi_0 \sin(\omega t - kx)$  ----- (1), Where  $\Psi = \Psi(x, t)$  and  $\Psi_0$  is the amplitude.

Differentiating  $\Psi$  partially w.r.to x,  $\partial \Psi / \partial x = \Psi_0 \cos(\omega t - kx) \cdot (-k)$

$$= -k \Psi_0 \cos(\omega t - kx)$$

Once again differentiate w.r.to x ,

$$\partial^2 \Psi / \partial x^2 = (-k) \cdot \Psi_0 (-\sin(\omega t - kx)) \cdot (-k)$$

$$= -k^2 \cdot \Psi_0 \sin(\omega t - kx)$$

$$\partial^2 \Psi / \partial x^2 = -k^2 \Psi \quad (\text{from equation (1)})$$

$$\partial^2 \Psi / \partial x^2 + k^2 \Psi = 0 \quad \text{----- (2)}$$

$$\partial^2 \Psi / \partial x^2 + (4\pi^2/\lambda^2) \Psi = 0 \quad \text{----- (3)} \quad (\text{since } k = 2\pi/\lambda)$$



From eqn. (2) or eqn. (3) is the differential form of the classical wave eqn. now we incorporate deBroglie wavelength expression  $\lambda = h / m v$ .

Thus, we obtain,  $\partial^2 \psi / \partial x^2 + (4 \pi^2 / (h / m v)^2) \psi = 0$

$$\partial^2 \psi / \partial x^2 + 4 \pi^2 m^2 v^2 \psi / h^2 = 0 \text{ ----- (4)}$$

The total energy E of the particle is the sum of its kinetic energy K and potential energy V

$$\text{i.e., } E = K + V \text{ ----- (5)}$$

$$\text{And } K = \frac{1}{2} m v^2 \text{ ----- (6)}$$

$$\text{Therefore } m^2 v^2 = 2 m (E - V) \text{ ----- (7)}$$

Substitute equation (7) in (4), we get

$$\Rightarrow \partial^2 \psi / \partial x^2 + [8 \pi^2 m (E - V) / h^2] \psi = 0 \text{ ----- (8)}$$

In quantum mechanics,  $\hbar = h / 2 \pi$

$$\partial^2 \psi / \partial x^2 + [2 m (E - V) / \hbar^2] \psi = 0 \text{ ----- (9)}$$

This is the One Dimensional Schrödinger Time Independent Wave Equation along x-axis.

Extending eqn. (9) for a two - dimensional, we get

$$\partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2 + [2 m (E - V) / \hbar^2] \psi = 0 \text{ ----- (10)}$$

Extending eqn. (9) for a three - dimensional, we get

$$\partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2 + \partial^2 \psi / \partial z^2 + [2 m (E - V) / \hbar^2] \psi = 0 \text{ ----- (11)}$$

Where  $\Psi = \Psi (x, y, z)$ .

Using the Laplacian operator,

$$\nabla^2 = \partial^2 / \partial x^2 + \partial^2 / \partial y^2 + \partial^2 / \partial z^2 \text{ ----- (12)}$$

$$\text{Eqn. (11) can be written as , } \nabla^2 \Psi + [2 m (E - V) / \hbar^2] \Psi = 0 \text{ ----- (13)}$$

This is the Three Dimensional Schrödinger Time Independent Wave Equation along x , y and z axes.

### \*Physical Significance of a Wave function ( $\Psi$ ) :-

Wave function ( $\Psi$ ):-It is the variable quantity that is associated with a moving particle at any position (x, y, z) at any

time 't'.

1. The wave function of a particle is represented by  $\Psi = \Psi_0 e^{-iEt/\hbar}$  or  $\Psi(x,y,z,t) = \Psi_0 e^{-i(\omega t - kx)}$

2. Wave function ( $\Psi$ ) explains the motion of microscopic particles.

3. Wave function ( $\Psi$ ) gives the information about the particle behaviour.

Wave function ( $\Psi$ ) is a complex quantity and it does not have any meaning.

4.  $|\Psi|^2 = \Psi\Psi^*$ , is real and positive. It has physical meaning. m

5.  $|\Psi|^2$  represents the probability of finding the particle per unit volume.

6. For a given volume  $d\Gamma$ , the probability of finding the particle is given by,

$$\text{Probability density (P)} = \iiint |\Psi|^2 d\Gamma, \text{ where } d\Gamma = dx dy dz.$$

7. If  $P = 0$ , then there is no chance for finding the particle i.e, there is no particle, within the given limits.

8. IF  $P=1$ , then there is 100% chance for finding the particle .i.e, the particle is definitely present ,within the given limits.

9. If  $P=0.7$ , Then there is 70% chance for finding the particle and 30% no chance for finding the particle.

10. 'P' values are between 0 to 1.

11. Wave function ( $\Psi$ ) is a single valued, finite and periodic function.

12. If  $P = \iiint |\Psi|^2 d\Gamma = 1$ , then ' $\Psi$ ' is called normalized wave function.

### LIMITATIONS OF A WAVE FUNCTION ( $\Psi$ ) :-

There are certain limitations to take ' $\Psi$ ' as a solution for the Schroedinger wave equation. They are,

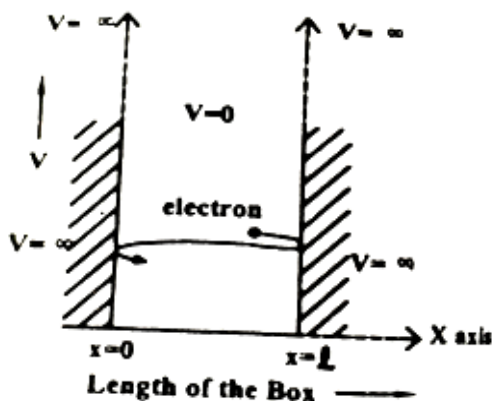
1. Wave function must be finite for all values of x,y,z.

2. Wave function must be single valued i.e, for each set of values of  $x, y$  &  $z$ .
3. Wave function must be continuous.
4. Wave function is analytical, i.e, it passes continuous first order derivative.
5. Wave function vanishes at the boundaries.

### \*\*\*APPLICATION OF SCHRODINGER TIME INDEPENDENT WAVE EQUATION:-

#### 1. A PARTICLE (OR) ELECTRON IN ONE DIMENSIONAL INFINITE SQUAREWELL POTENTIAL BOX:-

Let  
in a  
in  
the  
i.e,  
the



us consider a particle or electron of mass ' $m$ ' moving along X-axis, enclosed one dimensional potential box as shown figure.

Since the walls are of infinite potential, particle does not penetrate out from the box.

potential energy of the particle  $V = \infty$  at walls.

The particle is free to move between the walls A&B at  $x=0$  and  $x=L$ . The potential energy of the particle between the two walls is constant because no force is acting on the particle.

Therefore the potential energy is taken as zero for simplicity.

i.e,  $V = 0$  between  $x=0$  and  $x = L$ .

#### Boundary Conditions:-

The potential energy is,  $V(x) = 0$ , when  $0 < x < L$

$$V(x) = \infty, \text{ when } 0 \geq x \geq L$$

$$\Psi(x) = 0 \text{ at } x = 0$$

$$\Psi(x) = 0 \text{ at } x = L$$

The Schrödinger one - dimensional time independent equation of the particle along x-axis is given by,

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

For freely moving particle between the walls,  $V = 0$

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2m}{h^2} E\Psi = 0 \text{-----(1)}$$

$$\text{Consider, } \frac{8\pi^2m}{h^2} E = K^2$$

Then equation(1) becomes,

$$\frac{d^2\Psi}{dx^2} + K^2\Psi = 0 \text{ -----(2)}$$

The general solution of above equation is given by,

$$\Psi(x) = A \sin kx + B \cos kx \text{ -----(4), where A, B are two constants and k is a propagation constant (or) wave vector.}$$

Applying boundary conditions for equation(4), we get

$$(i). \Psi(x) = 0 \text{ at } x = 0$$

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

$$\Rightarrow 0 = A \sin k(0) + B \cos k(0)$$

$$\Rightarrow 0 = 0 + B$$

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

$$\text{Substitute 'B' value in equation(4), we get, } \Psi(x) = A \sin kx \text{ -----(5)}$$

$$(ii). \Psi(x) = 0 \text{ at } x = L$$

Then equation(5) becomes,  $\Psi(x) = A \sin kx$

$$\Rightarrow 0 = A \sin kL$$

But  $A \neq 0$ , and  $\sin kL = 0$

$$\Rightarrow \sin kL = \sin n\pi$$

$$\Rightarrow kL = n\pi$$

$$\text{Therefore, } k = \frac{n\pi}{L} \text{ -----(6)}$$

Substitute equation (6) in (5), we get

$$\Psi(x) = A \sin\left(\frac{n\pi}{L}x\right) \text{ -----(6)}$$

To find the 'A' value, apply the normalization condition:-

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

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

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

$$\Rightarrow A^2 \cdot \frac{L}{2} = 1$$

$$\Rightarrow A^2 = \frac{2}{L}$$

$$\Rightarrow A = \sqrt{\frac{2}{L}} \text{ -----(7)}$$

Substitute equation (7) in (6), we get

$$\Psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L}x \text{ (or) } \Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \text{ -----(8)}$$

*This is the normalized wave function of electron.*

Energy of the Electron:-

$$\text{From equation (6), } K = \frac{n\pi}{L} \Rightarrow K^2 = \frac{n^2\pi^2}{L^2}$$

$$\text{We have, } K^2 = \frac{8\pi^2 mE}{h^2}$$

$$\text{Then, } \frac{n^2\pi^2}{L^2} = \frac{8\pi^2 mE}{h^2}$$

$$\Rightarrow E_n = \frac{n^2 h^2}{8mL^2} \text{ -----(9)}$$

Therefore, *the energy (or) energy eigen function of the electron*,  $E_n = \frac{n^2 h^2}{8mL^2}$  (or)  $E_{n_x} = \frac{n_x^2 h^2}{8mL^2}$

Energy levels of an Electron:-

$$\text{The energy of the electron, } E_n = \frac{n^2 h^2}{8mL^2}$$

$$\text{When } n=1, E_1 = \frac{h^2}{8mL^2}$$

$$\text{When } n=2, E_2 = \frac{4 \cdot h^2}{8mL^2} = 4 \cdot E_1$$

$$\text{When } n=3, E_3 = \frac{9 \cdot h^2}{8mL^2} = 9 \cdot E_1$$

-----

In general,  $E_n = n^2 \cdot E_1$

*Therefore, the particle (electron) in the box has discrete values of energies. These values are quantized .*

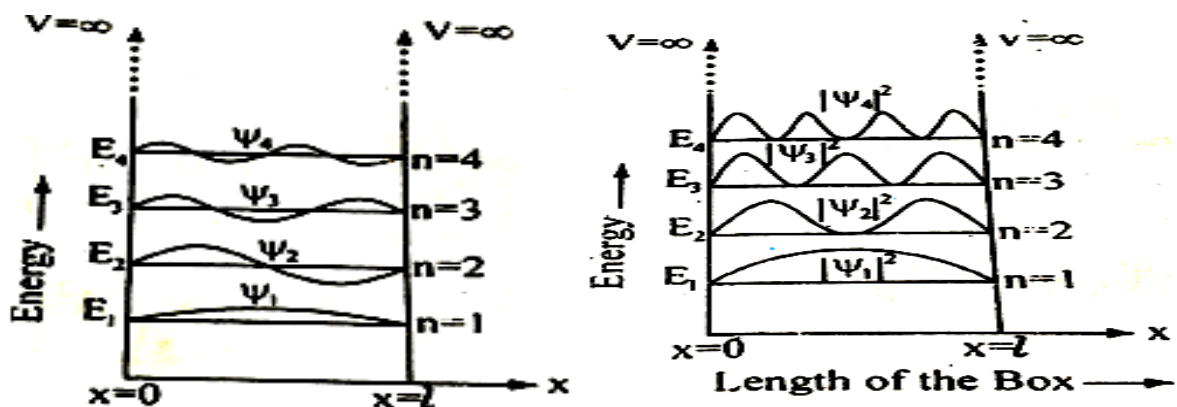
The normalized wave functions  $\Psi_1, \Psi_2, \Psi_3$ , electron probability densities  $|\Psi_1|^2, |\Psi_2|^2, |\Psi_3|^2, |\Psi_4|^2, \dots$ ,

energy eigen function  $E_n$  and their corresponding Eigen values  $E_1, E_2, E_3, E_4$ , are plotted, as shown in fig.

The wave function  $\Psi_1$ , has two nodes at  $x = 0$  &  $x = L$

The wave function  $\Psi_2$ , has three nodes at  $x = 0$ ,  $x = L/2$  &  $x = L$

The wave function  $\Psi_3$ , has three nodes at  $x = 0$ ,  $x = L/3$ ,  $x = 2L/3$  & at  $x = L$



## 2. A PARTICLE (OR) ELECTRON IN THREE DIMENSIONAL POTENTIAL BOX:

Normalized wave function of electron in three dimensional potential box is,

$$\begin{aligned} \Psi_n(x) \cdot \Psi_n(y) \cdot \Psi_n(z) &= \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \cdot \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi y}{L}\right) \cdot \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi z}{L}\right) \\ &= \left(\sqrt{\frac{8}{L^3}}\right) \cdot \sin\left(\frac{n\pi x}{L}\right) \cdot \sin\left(\frac{n\pi y}{L}\right) \cdot \sin\left(\frac{n\pi z}{L}\right) \end{aligned}$$

The energy (or) energy eigen function of the electron

$$E_{n_x} \cdot E_{n_y} \cdot E_{n_z} = \frac{(n_x^2 + n_y^2 + n_z^2)h^2}{8mL^2}$$

$$\text{In general, the energy of electron} = E_n = \frac{n^2 h^2}{8mL^2}$$

## DEGENERATE AND NON DEGENERATE STATES:-

Degenerate States: -The energy states which have the same energy eigen value (or) energy functions but different eigen functions, such states are called as degenerate states (or) levels.

Non degenerate States:- The energy states which have the same energy eigen value (or) energy functions and the same eigen functions, such states are called as non degenerate states.

Differences between Matter wave and Electro Magnetic wave:-

Matter wave	ElectroMagnetic (EM) wave
1) Matter wave is associated with moving particle	1)Oscillating charged particle gives rise to EM wave.
2) wavelength, $\lambda = h/mv$	2) Wavelength, $\lambda = hc/E$ .
3) Wavelength depends on the mass of the particle & its velocity.	3) Wavelength depends on the energy of the photon.
4) It can travel with a velocity greater than the velocity of light.	4) it travels with velocity of light $c= 3 \times 10^8$ m/s
5) It is not a electromagnetic wave.	5) Electric field and magnetic field oscillate perpendicular to each other.

### SOLVED PROBLEMS:

Example.1 *Calculate the wavelength associated with an electron raised to a potential of 400V.*

Principle:  $\lambda = \frac{12.27}{\sqrt{V}} \text{ \AA}$

Solution : :  $\lambda = \frac{12.27}{\sqrt{400}} \text{ \AA} = 0.6135 \text{ \AA}$



Example.2 An electron is confined to a one dimensional potential box of length  $2 \text{ \AA}$ . Calculate the energies corresponding to the second and fourth quantum states (in eV).

Given Data : Potential box length .  $L = 2 \text{ \AA} = 2 \times 10^{-10} \text{ m}$

Second quantum state ,  $n = 2$

Fourth quantum state ,  $n = 4$

Energy of second  $E_2 = ?$

Energy of second  $E_4 = ?$

$$\text{Principle : } E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{h^2 n^2}{8mL^2}$$

Solution : For  $n=2$  ,

$$E_2 = \frac{4 \times (6.626 \times 10^{-34})^2 \text{ J-Sec}}{8 \times 9.1 \times 10^{-31} \text{ kg} \times 2 \times 10^{-10} \text{ m}}$$

$$E_2 = 0.812 \times 10^7 \text{ J}$$

$$E_2 = \frac{0.812 \times 10^7}{1.6 \times 10^{-19}} \text{ eV} = 0.1137 \times 10^{26} \text{ eV}$$

For  $n= 4$ ,

$$E_4 = \frac{16 \times (6.626 \times 10^{-34})^2 \text{ J-Sec}}{8 \times 9.1 \times 10^{-31} \text{ kg} \times 2 \times 10^{-10} \text{ m}}$$

$$E_4 = 0.728 \times 10^7 \text{ J}$$

$$E_4 = \frac{0.728 \times 10^7}{1.6 \times 10^{-19}} \text{ eV} = 0.455 \times 10^{26} \text{ eV}$$

Example.3

What is the wavelength in meters of a proton traveling at 255,000,000 m/s (which is 85% of the speed of light)? (Assume the mass of the proton to be  $1.673 \times 10^{-27} \text{ kg}$ .)

1) Calculate the kinetic energy of the proton:

$$\text{KE} = (1/2)mv^2$$

$$x = (1/2) (1.673 \times 10^{-27} \text{ kg}) (2.55 \times 10^8 \text{ m/s})^2 = 5.43934 \times 10^{-11} \text{ J}$$

2) Use the de Broglie equation:  $\lambda = h/p$  ,  $\lambda = h/\sqrt{2Em}$

$$\lambda = 6.626 \times 10^{-34} \text{ J s} / \sqrt{[(2) (5.43934 \times 10^{-11} \text{ J}) (1.673 \times 10^{-27} \text{ kg})]}$$

$$\lambda = 1.55 \times 10^{-15} \text{ m}$$

This wavelength is comparable to the radius of the nuclei of atoms, which range from  $1 \times 10^{-15} \text{ m}$  to  $10 \times 10^{-15} \text{ m}$

(or 1 to 10 fm).

## Questions:

What are the matter waves? Explain their properties.

Explain de Broglie hypothesis.

Explain the duality of matter waves

Describe Davisson and Germer's experiment and explain how it enabled the verification of the de Broglie equation.

Explain G.P. Thompson's experiment in support of de Broglie hypothesis

Explain Heisenberg's uncertainty principle. Give its physical significance.

Derive time independent one dimensional Schrödinger's equation.

Explain the physical significance of wave function.

Write down Schrödinger's wave equation for a particle in one dimensional potential box.