

# 4

## QUANTUM PHYSICS

### 4.1 INTRODUCTION

Newtonian mechanics, Maxwell's electromagnetic theory and thermodynamics guided the growth of science and engineering during the years spanning 17<sup>th</sup> to 19<sup>th</sup> centuries.

The theories explained almost all the scientific results of those times and it seemed nothing more could be added. The above theories which are successful in the realms of macroscopic world are regarded as **classical physics**.

In the classical physics, matter and fields are treated as entirely independent entities. Macroscopic particles move and interact according to Newton's laws.

- i) The physical quantities such as **particle energy** are continuously variable and take any possible value. For example, the potential energy of a body falling freely in the gravitational field decreases continuously from a specific value ' $mgh$ ' at a height ' $h$ ' to zero as it touches the ground.

- ii) If the state of a particle is known at a particular instant and if the forces acting on the particle at that instant are known, the state of the particle at any future instant can be exactly predicted. Thus, if we know the initial position and velocity of a freely falling body, we can exactly predict its position and velocity at any other instant meaning thereby that the particle follows a definite trajectory.
- iii) A particle can be isolated from its environment and can be treated as an independent entity for the investigation. Thus the particles under investigation and the instrument measuring any of its parameters are mutually independent.

According to classical wave theory,

- i) Electromagnetic waves are generated by accelerated charges; if a charge oscillates with a constant frequency  $\nu$ , it produces an electromagnetic wave of same frequency  $\nu$ .
- ii) The waves spread out continuously through space and the wave energy is not localized; but is distributed over the volume of the wave.
- iii) The energy of the wave is not related to the frequency of the wave. It is proportional to the square of the amplitude  $A$  of the wave i.e.,  $I \propto |A|^2$ .
- iv) The thermodynamic equilibrium of an assembly of neutral particles is governed by Maxwell-Boltzmann statistics. A large number of particles can occupy a given energy state and the particles can have a continuous range of energies.

During the end of 19<sup>th</sup> century, a number of new phenomena such as photoelectric effect, x-rays, line spectra, ultraviolet catastrophe and radioactivity were discovered which could not be explained on the basis of classical physics. A search for correct solutions led the scientists to abandon old ideas and devise new concepts.

The inadequacy of classical physics is well understood when it is applied to the Rutherford model of the atom. According to this model, the atom is composed of a tiny, massive, positively charged nucleus around which negatively charged electrons revolve.

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The atom is mechanically stable as the coulomb attractive force between the nucleus and the electrons is balanced by the centripetal force.

However, according to electromagnetic theory, the accelerated electron should radiate energy in the form of electromagnetic waves. If electron radiates energy, its own energy gets reduced. It therefore gradually spirals into the nucleus leading to the ultimate collapse of the atom. It means that atoms are unstable and exist only for a fraction of a second.

Secondly, they should emit a continuous spectrum. In reality atoms are highly stable and give line spectra. Thus, classical physics fails to provide a satisfactory model for the structure of the atom and its stability.

The debacle of classical physics in such cases indicates that the classical laws are not valid in the microscopic world. The microworld of atoms obey different laws. The new laws applicable for microparticles constitute quantum mechanics.

The revision of classical concepts was begun with the seminal hypothesis of Planck and many distinguished physicists such as Einstein, Bohr, de Broglie, Schrodinger, Born, Pauli, Heisenberg, Dirac and others contributed to the development of quantum mechanics.

### **4.2 ULTRAVIOLET CATASTROPHE**

It is a matter of common experience that when a body is heated it emits radiation. The radiation emitted by hot bodies is called **thermal radiation**. Even at ordinary temperatures a body emits radiation over a range of frequencies.

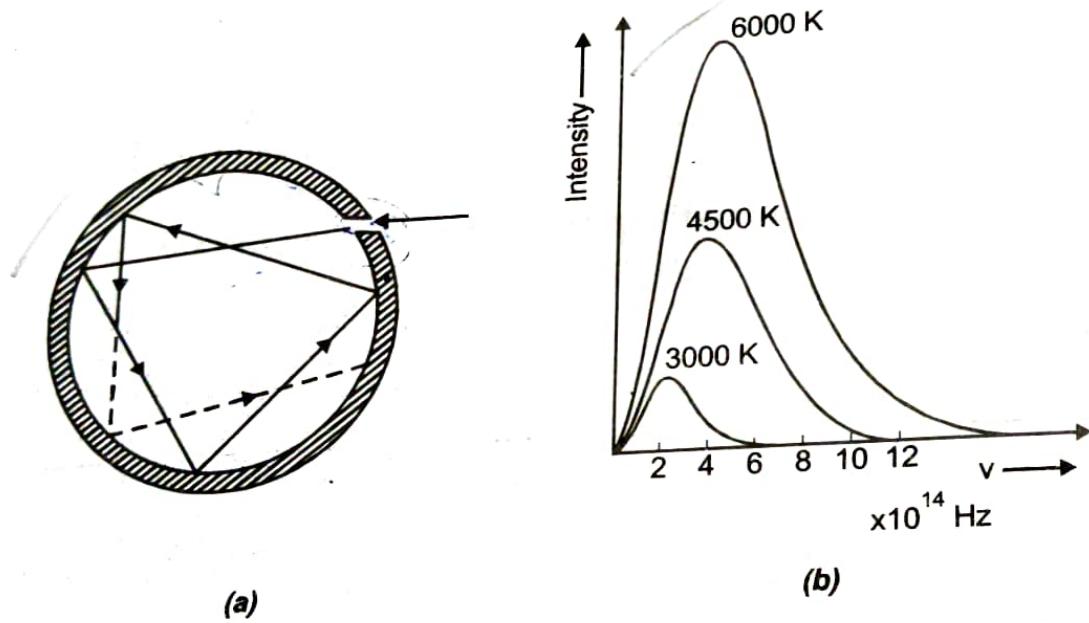
The relative brightness of the different frequencies depends on the temperature of the body. As the temperature of the body is increased, the component of maximum intensity shifts to a higher and higher frequency.

For example, an iron rod appears dark at ordinary temperatures and when heated it appears faint crimson at around  $500^{\circ}\text{C}$ , then turns red-orange gradually and yellow at  $800^{\circ}\text{C}$ . Finally it emits white light above  $1000^{\circ}\text{C}$ . 

The thermal radiation emitted by an idealized body called a **black body** (Figure 4.1(a)) was thoroughly analysed using spectrographs and bolometers.

The experimental results, illustrated in figure 4.1(b) showed that at a given temperature the radiation energy density initially increases with frequency, then peaks at around a particular frequency and after that decreases finally to zero at very high frequencies.

Various efforts were made to theoretically calculate the frequency distribution of thermal radiation using Maxwell's electromagnetic wave theory and thermodynamics.



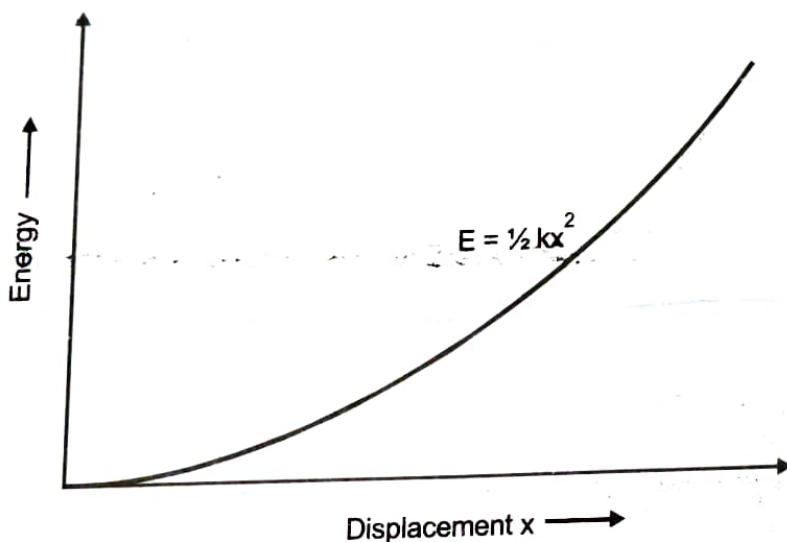
(a) A black body: a black body absorbs all light and reflects none of the light incident on it. A spherical cavity blackened inside and completely closed except a narrow aperture serves as an ideal black body. Light entering the cavity is trapped inside by multiple reflections from the walls. When heated, the black body would emit more from a unit area than any other body at a given temperature.

(b) Spectral energy distribution of black body radiation. Area under a curve represents the total radiation emitted by a black body at a given temperature. Note that the area increases rapidly with rising temperature and the peak frequency is displaced towards higher frequency. This is why a hot body, for example the filament in an electric bulb, changes from red through orange to white with a rise in temperature.

Fig. 4.1

In these theories, a body was assumed to consist of a huge number of atoms each of which acts as a generator of radiation. It was assumed that each atom absorbs energy continuously from the source and oscillates at its own frequency leading to emission of a continuous spectrum of wavelengths.

The energy is absorbed and emitted by atomic oscillators in every conceivable amount, from zero upto some maximum value, as illustrated in figure 4.2.



**Fig. 4.2: A classical oscillator such as a spring can have any amount of energy from zero to some maximum value and the energy distribution is continuous.**

The classical theory based on the above concepts predicted that the intensity of thermal radiation should increase with square of frequency ( $v^2$ ). The theory agrees with experimental results at lower frequencies but leads to absurd result at higher frequency end.

The theory implies that the radiation emitted by a hot body should have a large portion of UV rays. This is contrary to our experience and clearly violates the law of conservation of energy. This contradiction is called the ultraviolet catastrophe. Thus, classical theories of physics failed to explain the distribution of thermal radiation emitted by solid bodies.

In 1884 Stefan and Boltzmann had shown that the energy of radiation in unit volume of space due to all the different wavelengths in the spectrum was proportional to the fourth power of the absolute temperature of the black body which is well known as Stefan's fourth power law.

From thermodynamical considerations, Wien in 1893 showed that the product of the wavelength corresponding to maximum energy ( $\lambda_m$ ) and absolute temperature is a constant i.e.,  $\lambda_m T = \text{a constant}$ .

This is known as **Wien's displacement law**. He also showed that the maximum energy  $E_m \propto T^5$  or  $E_m = \text{constant} \times T^5$

He also deduced the radiation law for energy emitted at a particular wavelength  $\lambda$  and given temperature  $T$  as

$$E_\lambda = C_1 \lambda^{-5} \exp\left(\frac{-C_2}{\lambda T}\right)$$

where  $C_1$  and  $C_2$  are constants.

This formula holds good only for shorter wavelengths.

Note that in the above formula even when  $T = \infty$ ,  $E$  is still finite, which is in open contradiction to the experimentally verified Stefan's fourth power law.

### Rayleigh Jean's law

In 1900 Rayleigh and Jeans using electromagnetic theory, statistical and classical mechanics showed that the energy distribution of the black body can be given by

$$E_\lambda = \frac{8\pi kT}{\lambda^4}$$

Here,  $k$  is the Boltzmann's constant.

This formula agrees well for longer wavelengths only.

Again in the above formula, the energy radiated in a given wavelength range  $d\lambda$  increases rapidly as  $\lambda$  decreases and approaches infinity for very short wavelengths which is not true. Further if the expression is integrated over the whole range of wavelengths from 0 to  $\infty$  on the basis of classical continuous emission, the total energy obtained turns out to be infinite for all temperatures except absolute zero, which is clearly absurd.

Hence we see that no theoretical formulae could account for the shape of the radiation curve over the entire wavelength range.

However since the theoretical derivations were free from error, an anomalous situation had to be accepted in the disagreement of theory with experiment, unless one **assumed** that the fundamental assumptions of the **classical theory** were at fault.

This was what exactly occurred to **Planck** who in 1901 proposed a new **revolutionary hypothesis** known as the **theory of quanta** by which he was able to derive the correct law of **thermal radiation**.

### Planck's Theory of Quanta

Planck's chief aim was to make theory fit with experimental facts. Planck argued that the classical idea of continuity of action might be wrong and proposed instead that the energy changes could take place only **discontinuously and discretely**, always as integral multiples of a small unit called **quantum**. With this statement, the quantum theory came into being, although **Planck** himself did not realise then the far reaching consequences of his new idea. He was intent on getting a correct radiation law.

He assumed that the cavity of an experimental black body was filled with electrical linear oscillators of the **Hertzian type**, since such oscillators had been shown to give a final confirmation to the electromagnetic theory by their actual production of electromagnetic waves.

Radiation emitted by the oscillators would eventually fill the cavity and reach equilibrium at some definite temperature, when radiation would be both absorbed and emitted by each oscillator.

Under these conditions, any oscillator would affect only radiation of the same frequency as that of itself and in consequence there would be a definite ratio between the density of radiation of any given frequency and the average energy of the oscillators at that frequency.

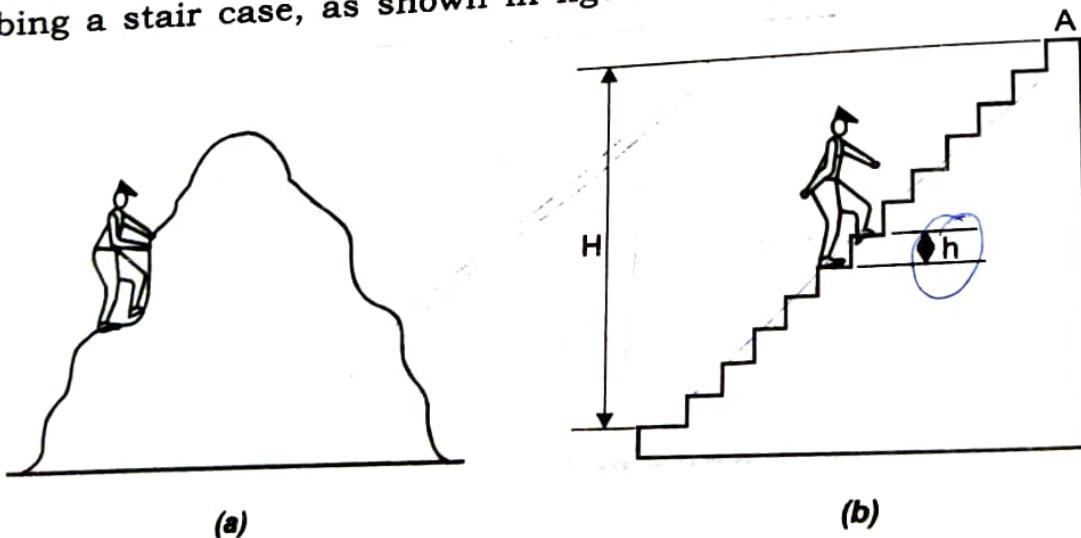
In this way the problem of spectral distribution of radiant energy present in the cavity could be reduced to that of the average energy of an oscillator at a given temperature.

Next, using the quantum idea, he supposed that the linear oscillators can vibrate only with integral energy values  $0, \varepsilon, 2\varepsilon, \dots n\varepsilon$ , where ' $\varepsilon$ ' represents the elementary quantum.

He assumed that ' $\varepsilon$ ' was proportional to  $1/\lambda$  or to ' $v$ ' so that  $\varepsilon = hv$ .

He found the expression for the average energy per oscillator and multiplied it by the effective number of independent resonating modes of frequency ' $v$ ' per unit volume in the cavity which would give the energy density. The formula matched the experimental curves excellently.

Max Planck was honoured in 1918 with a Nobel Prize in Physics. The quantum concept can be understood with the help of the following example. Consider a person walking up a hill and another person climbing a stair case, as shown in figure 4.4.



**Fig. 4.4: Examples of a continuous change and discrete change in energy; (a) the potential energy increases (or decreases) in a continuous manner and through arbitrary amounts as a person climbs (or descends) the hill; (b) the potential energy increase (or decreases) in fixed steps of ' $mgh$ ' as a person climbs (or descends) the steps of a stair case.**

Both of them gain potential energy. The potential energy of the person going up the hill increases **continuously** through **arbitrary** amounts of energy. In contrast, the potential energy of the person climbing the stair case increases in a discrete manner through a fixed amount of energy. If all the steps are assumed to be of the same height ' $h$ ', the person acquires a quantum of energy ' $mgh$ ' each time he goes by one step.

Consequently, his potential increases by  $1 \text{ mgh}$ ,  $2 \text{ mgh}$ ,  $3 \text{ mgh}$ ..... $N \text{ mgh}$ . It is not possible to acquire an energy which is a fraction of  $\text{mgh}$  or of any intermediate value.

While getting down the hill, a person loses energy in a continuous manner and while getting down the steps, a person loses energy in steps of  $\text{mgh}$ .

With the above introduction let us now proceed to derive the **Planck's Radiation law**.

### Derivation of Planck's Radiation Law

#### Planck's Hypothesis

1. The chamber containing the black body consists of a number of oscillators (simple harmonic) of atomic/molecular dimensions and can vibrate with all possible frequencies.
2. The frequency of vibration of an oscillator is the same as the frequency of radiation emitted by it.
3. An oscillator cannot emit energy in a continuous manner. It can emit energy only in multiples of a small unit called **quantum**. If an oscillator vibrates with a frequency ' $v$ ' it can only radiate in **quanta** of magnitude  $hv$  (where ' $h$ ' is the Planck's constant). The oscillator can have only discrete energy values.

$$\text{i.e., } E_n = n h v = n \epsilon$$

where  $n$  is a integer. ( $h v = \epsilon$ )

4. The oscillators can emit or absorb radiation only in packets of ' $\epsilon$ '. This implies that exchange of energy between radiation and matter cannot take place continuously but is limited to a discrete set of values  $0, hv, 2hv, \dots$  (i.e.,  $0, \epsilon, 2\epsilon, \dots$ )

Now in a black body, there are a number of oscillators of frequencies  $v_1, v_2, \dots$ . We are interested in finding the energy density for a particular frequency range ' $v$  to  $v + dv$ ' which may be due to a number of oscillators vibrating with **frequency 'v'** and its **harmonics**. So our problem now is to find the **average energy** of such oscillators.

Let there be 'N' number of such Planck's oscillators and 'E' be their total energy.

∴ The average energy per Planck's oscillator

$$\bar{\varepsilon} = \frac{E}{N} \quad \dots (1)$$

Let there be  $N_0, N_1, N_2, \dots, N_r$ .

Oscillators having energy  $0, \varepsilon, 2\varepsilon, \dots, r\varepsilon$ .

$$\therefore N = N_0 + N_1 + N_2 + \dots + N_r + \dots \quad \dots (2)$$

$$\text{and } E = 0 + \varepsilon N_1 + 2\varepsilon N_2 + 3\varepsilon N_3 + \dots + r\varepsilon N_r + \dots \quad \dots (3)$$

Now using Maxwell Boltzmann's distribution, the number of oscillators having energy  $r\varepsilon$  is given by

$$N_r = N_0 \exp\left(\frac{-r\varepsilon}{kT}\right) \quad \dots (4)$$

where 'k' is the Boltzmann's constant.

Substituting the values of  $N_1, N_2, N_3, \dots$  from (4) in (2), we get,

$$\begin{aligned} N &= N_0 + N_0 \exp\left(\frac{-\varepsilon}{kT}\right) + N_0 \exp\left(\frac{-2\varepsilon}{kT}\right) + \dots + N_0 \exp\left(\frac{-r\varepsilon}{kT}\right) + \dots \\ \Rightarrow N &= N_0[1 + x + x^2 + \dots + x^r + \dots] \end{aligned} \quad \dots (5)$$

where  $x = \exp\left(\frac{-\varepsilon}{kT}\right)$

$$\Rightarrow N = \frac{N_0}{(1-x)} \quad \left[ \text{As } 1 + x + x^2 + \dots = \frac{1}{(1-x)} \right] \quad \dots (6)$$

Applying (4) in (3), we obtain,

$$\begin{aligned} E &= (N_0 0) + \varepsilon N_0 \exp\left(\frac{-\varepsilon}{kT}\right) + 2\varepsilon N_0 \exp\left(\frac{-2\varepsilon}{kT}\right) \\ &\quad + 3\varepsilon N_0 \exp\left(\frac{-3\varepsilon}{kT}\right) + \dots + r\varepsilon N_0 \exp\left(\frac{-r\varepsilon}{kT}\right) + \dots \end{aligned}$$

$$= N_0 \varepsilon x [1 + 2x + 3x^2 + 4x^3 + \dots + rx^{r-1} + \dots] \quad \dots (7)$$

Where  $x = \exp\left(\frac{-\varepsilon}{kT}\right)$

$$E = N_0 \varepsilon x \left[ \frac{1}{(1-x)^2} \right] \quad \dots (8)$$

$$\left[ \text{As } 1+2x+3x^2+4x^3+\dots = \frac{1}{(1-x)^2} \right]$$

From (6) and (8), we have the average energy of an oscillator,

$$\bar{\varepsilon} = \frac{E}{N} = \frac{N_0 \varepsilon x \left[ \frac{1}{(1-x)^2} \right]}{N_0/(1-x)}$$

$$\Rightarrow \bar{\varepsilon} = \frac{\varepsilon \exp\left(\frac{-\varepsilon}{kT}\right)}{1 - \exp\left(\frac{-\varepsilon}{kT}\right)}$$

$$\Rightarrow \bar{\varepsilon} = \frac{\varepsilon}{\frac{1}{\exp\left(\frac{-\varepsilon}{kT}\right)} - \frac{\exp(-\varepsilon/kT)}{\exp(-\varepsilon/kT)}}$$

$$\Rightarrow \bar{\varepsilon} = \frac{\varepsilon}{\exp\left(\frac{\varepsilon}{kT}\right) - 1} \quad \dots (9)$$

$$\Rightarrow \bar{\varepsilon} = \frac{h\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1} \quad \dots (10)$$

Equation (9) and (10) give the average energy of an oscillator which is totally different from the value ( $kT$ ) of a classical oscillator.

In equation (9) if ' $\epsilon$ ' is small.

$$\exp\left(\frac{\epsilon}{kT}\right) = \left(1 + \frac{\epsilon}{kT}\right)$$

and  $\epsilon = \frac{\epsilon}{1 + \frac{\epsilon}{kT} - 1} = kT$

the value for a classical oscillator.

It can be shown that the number of oscillators per unit volume in the frequency range ' $v$  to  $v + dv$ ' is

$$N' = \frac{8\pi v^2 dv}{c^3} \quad \dots (11)$$

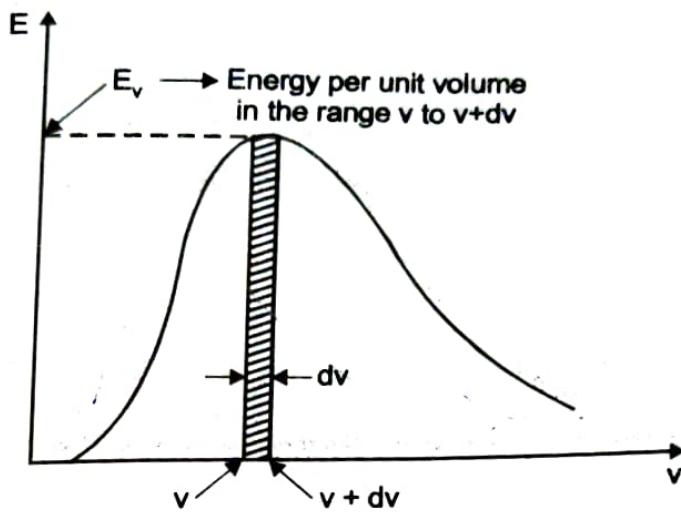
Multiplying equation (11) with the average energy of an oscillator i.e., equation (10), we get the total energy per unit volume belonging to the range ' $dv$ ' or the energy density belonging to the range ' $dv$ ' is

$$E_v dv = \frac{8\pi v^2 dv}{c^3} \left( \frac{hv}{\exp\left(\frac{hv}{kT}\right) - 1} \right)$$

$$E_v dv = \frac{8\pi hv^3}{c^3} \left( \frac{1}{\exp\left(\frac{hv}{kT}\right) - 1} \right) dv \quad \dots (12)$$

This equation (12) is known as **Planck's radiation law**. The above equation implies that taking the range ( $v$  to  $v + dv$ ), the portion of the curve shown in the below figure can be built up for a particular temperature.

The whole curve can be built up for the entire range of frequency ranges for a particular temperature.



In terms of ' $\lambda$ '

$$\text{As } v = \frac{c}{\lambda} \text{ and } |dv| = \left| \frac{-c}{\lambda^2} d\lambda \right|$$

$$\checkmark = \frac{c}{\lambda} \quad = \frac{c}{\lambda^2} d\lambda$$

$$E_\lambda d\lambda = \frac{8\pi hc^3}{c^3 \lambda^3} \left( \frac{1}{\exp\left(\frac{hc}{\lambda kT}\right)} \right) \frac{c}{\lambda^2} d\lambda$$

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \left( \frac{1}{\exp\left(\frac{hc}{\lambda kT}\right) - 1} \right) d\lambda$$

$$\begin{aligned} dv &= -\frac{c}{\lambda^2} d\lambda \\ &= \frac{c}{\lambda} d\lambda \\ (\checkmark &= c/\lambda) \\ dv &= c d\lambda \end{aligned}$$

.. (13)

The above formulae i.e.,  $E_v dv$  and  $E_\lambda d\lambda$  agree well for the whole radiation curve.

### 1. Deduction of Wien's formula from Planck's radiation formula

For short wavelengths,

$$\exp\left(\frac{hc}{\lambda kT}\right) \gg 1$$

Hence 1 may be neglected in comparison to  $\exp\left(\frac{hc}{\lambda kT}\right)$  in Planck's formula.

$$\therefore E_\lambda d\lambda = \frac{8\pi hC}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{\lambda kT}\right)} d\lambda$$

$$E_\lambda d\lambda = C_1 \lambda^{-5} \exp\left(\frac{-C_2}{\lambda T}\right) d\lambda$$

which is Wien's formula.

### 2. Deduction of Rayleigh-Jeans law from Planck's law

For longer wavelengths, i.e.,  $\nu$  small,  $\frac{h\nu}{kT}$  is small.

$$\therefore \exp\left(\frac{h\nu}{kT}\right) = 1 + \frac{h\nu}{kT} \text{ (neglecting higher powers)}$$

$$E_\lambda d\lambda = \frac{8\pi hC}{\lambda^5 \left[1 + \frac{h\nu}{kT} - 1\right]} d\lambda$$

$$E_\lambda d\lambda = \frac{8\pi hC kT}{\lambda^5 h\nu} d\lambda$$

$$E_\lambda d\lambda = \frac{8\pi kT}{\lambda^4} d\lambda$$

which is Rayleigh-Jeans law.

## 4.3 COMPTON EFFECT

### Statement

When a beam of high frequency radiation (X-ray or  $\gamma$ -ray) is scattered by a substance of low atomic number, the scattered radiation consists of two components, one has the same wavelength as the original incident ray and the other has a slightly longer wavelength. The phenomenon of change in the wavelength of scattered X-rays or  $\gamma$ -rays is called Compton shift and the effect is known as Compton effect. It was discovered by A.H.Compton in 1920.

### Explanation

Compton effect can be explained on the basis of quantum theory. An X-radiation consists of light quanta or photons each having energy  $h\nu$ . When a photon collides with a free electron of the scattering substance, it transfers some of the energy to the electron. As a result the scattered photon will have lower energy (lower frequency or longer wavelength) than that of the incident one.

### 4.3.1 Theory of Compton Effect

Consider an X-ray photon striking an electron, which is assumed to be **initially at rest** (Fig.4.5 a). The X-ray photon is scattered through an angle  $\theta$  from its initial direction of motion. Assume the collision to be elastic.

The electron receiving an impulse begins to move with a velocity  $v$  at an angle  $\phi$  from the direction of incident photon (Fig.4.5b).

### Energy before collision

$$\text{Initial energy of photon} = h\nu$$

where,  $h$  is Planck's constant and  $\nu$  is frequency.

$$\text{Initial energy of electron} = m_0 c^2$$

where,  $m_0$  is the initial rest mass of electron and  $c$  is the velocity of light.

$$\text{Total initial energy} = h\nu + m_0 c^2$$

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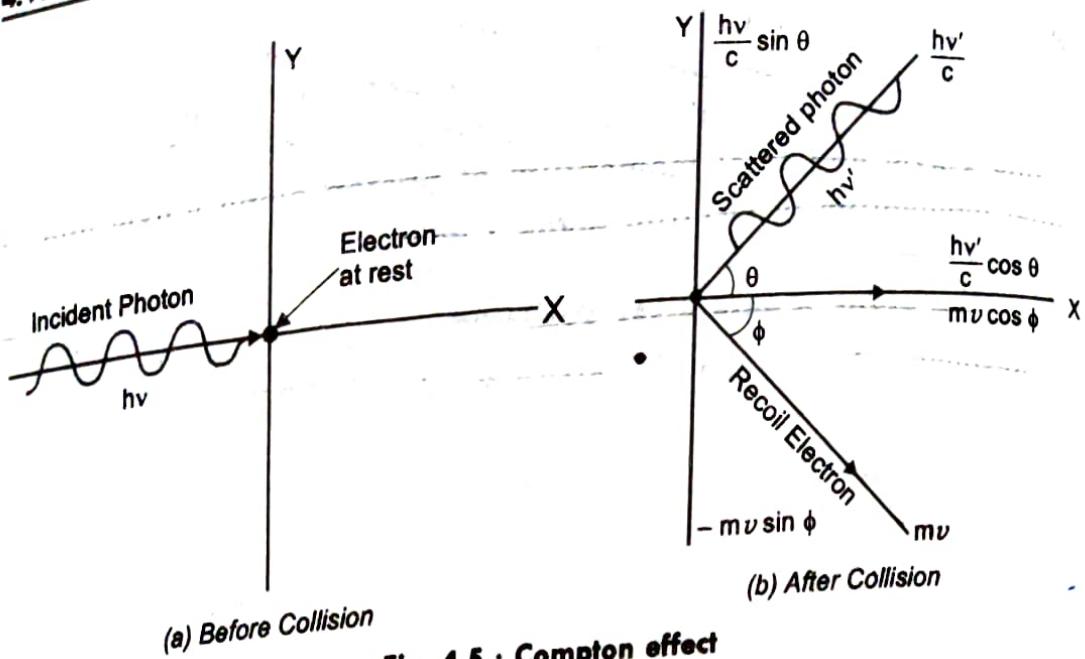


Fig. 4.5 : Compton effect

**Energy after Collision**

$$\text{Energy of scattered photon} = h\nu'$$

where  $\nu'$  is the scattered photon frequency.

$$\text{Energy of recoiled electron} = mc^2$$

where,  $m$  is the mass of electron, when in motion with a velocity ' $v$ '

$$\text{Total final energy} = h\nu' + mc^2$$

According to conservation of energy,

$$\text{Energy before collision} = \text{Energy after collision}$$

$$h\nu + m_0 c^2 = h\nu' + mc^2 \quad \dots (1)$$

**Momentum along x-axis before collision**

$$\text{Initial momentum of photon along } x\text{-axis} = \frac{h\nu}{c}$$

$$\text{Initial momentum of electron along } x\text{-axis} = 0$$

$$\text{Total initial momentum along } x\text{-axis} = \frac{h\nu}{c}$$

Since the momentum is a vector quantity it is resolved into x-axis components and y-axis components namely final momentum of photon along x-axis, final momentum of electron along x-axis and final momentum of photon along y-axis and final momentum of electron along y-axis.

### Momentum along x-axis after collision

Resolving the momentum along x-axis we have,

$$\text{Final momentum of photon along } x\text{-axis} = \frac{h\nu'}{c} \cos \theta$$

$$\text{Final momentum of electron along } x\text{-axis} = mv \cos \phi$$

$$\text{Total final momentum along } x\text{-axis} = \frac{h\nu'}{c} \cos \theta + mv \cos \phi$$

According to law of conservation of momentum

Momentum before collision along x axis	=	Momentum after collision along x axis
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$$\frac{h\nu}{c} = \frac{h\nu'}{c} \cos \theta + mv \cos \phi \quad \dots (2)$$

### Momentum along y-axis before collision

$$\text{Initial momentum of photon along } y\text{-axis} = 0$$

$$\text{Initial momentum of electron along } y\text{-axis} = 0$$

$$\text{Total initial momentum along } y\text{-axis} = 0$$

### Momentum along y-axis after collision

Resolving the momentum along y-axis we have

$$\text{Final momentum of photon along } y\text{-axis} = \frac{h\nu'}{c} \sin \theta$$

$$\text{Final momentum of electron along } y\text{-axis} = -mv \sin \phi$$

$$\text{Total final momentum along } y\text{-axis} = \frac{hv'}{c} \sin \theta - mv \sin \phi$$

According to law of conservation of momentum

$$\begin{array}{ccc} \text{Momentum before collision} & & \text{Momentum after collision} \\ \text{along } y\text{-axis} & = & \text{along } y\text{-axis} \end{array}$$

Momentum before collision along  $y$ -axis = Momentum after collision along  $y$ -axis

$$0 = \frac{hv'}{c} \sin \theta - mv \sin \phi \quad \dots (3)$$

Equation (2) is rewritten as

$$hv = hv' \cos \theta + mvc \cos \phi$$

$$h(v - v' \cos \theta) = mvc \cos \phi \quad \dots (4)$$

Equation (3) is rewritten as

$$hv' \sin \theta = mvc \sin \phi \quad \dots (5)$$

Squaring equations (4) and (5) and adding, we have

$$\begin{aligned} h^2(v^2 + v'^2 \cos^2 \theta - 2vv' \cos \theta + v'^2 \sin^2 \theta) &= m^2 v^2 c^2 (\cos^2 \phi + \sin^2 \phi) \\ h^2(v^2 + v'^2 - 2vv' \cos \theta) &= m^2 v^2 c^2 \end{aligned} \quad \dots (6)$$

From equation (1) we have,

$$hv + m_0 c^2 = hv' + mc^2$$

$$h(v - v') + m_0 c^2 = mc^2 \quad \dots (7)$$

Squaring the above equation we have,

$$h^2(v^2 - 2vv' + v'^2) + 2h(v - v') m_0 c^2 + m_0^2 c^4 = m^2 c^4 \quad \dots (8)$$

Subtracting equation (6) from (8) we get,

$$m^2 c^2 (c^2 - v^2) = -2h^2 vv'(1 - \cos \theta) + 2h(v - v') m_0 c^2 + m_0^2 c^4 \quad \dots (9)$$

According to Einstein's theory of relativity, we have

$$m = \frac{m_0}{\sqrt{\left(1 - \frac{v^2}{c^2}\right)}}$$

Squaring both sides,

$$m^2 = \frac{m_0^2}{1 - \frac{v^2}{c^2}} = \frac{m_0^2}{\frac{c^2 - v^2}{c^2}} = \frac{m_0^2 c^2}{c^2 - v^2}$$

$m^2(c^2 - v^2) = m_0^2 c^2$  multiplying  $c^2$  on both sides we get,

$$m^2 c^2 (c^2 - v^2) = m_0^2 c^4 \quad \dots (10)$$

Substituting equation (10) in equation (9) we have,

$$m_0^2 c^4 = -2h^2 vv'(1 - \cos \theta) + 2h(v - v')m_0^2 c^2 + m_0^2 c^4$$

$$2h(v - v')m_0 c^2 = 2h^2 vv'(1 - \cos \theta)$$

$$\frac{v - v'}{vv'} = \frac{h}{m_0 c^2} (1 - \cos \theta)$$

$$\frac{1}{v'} - \frac{1}{v} = \frac{h}{m_0 c^2} (1 - \cos \theta)$$

$$\frac{c}{v'} - \frac{c}{v} = \frac{h}{m_0 c} (1 - \cos \theta)$$

$$\lambda' - \lambda = \frac{h}{m_0 c} (1 - \cos \theta) \quad \left( \because \frac{c}{v'} = \lambda' \text{ and } \frac{c}{v} = \lambda \right)$$

Therefore, the change in wavelength is given by

$$d\lambda = \frac{h}{m_0 c} (1 - \cos \theta)$$

 $\dots (11)$

From the above expression we can come to a conclusion that the change in wavelength  $d\lambda$  is independent of the wavelength of the incident radiation as well as the nature of the scattering substance but depends on the angle of scattering  $\theta$ .

Also, as the limits of  $\cos \theta$  are from -1 to +1, the R.H.S of equation (11) is always positive. Hence  $d\lambda$  is positive which means  $\lambda' > \lambda$ . That is the scattered radiation has a longer wavelength.

**Case I:**

When  $\theta = 0$ ,  $\cos \theta = 1$  Hence,  $d\lambda = 0$

**Case II:**

When  $\theta = 90^\circ$ ,  $\cos \theta = 0$ , then

$$d\lambda = \frac{h}{m_e c} = \frac{6.625 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} = 0.0243 \text{ Å}$$

This is known as **Compton wavelength** of electron.

**Case III:**

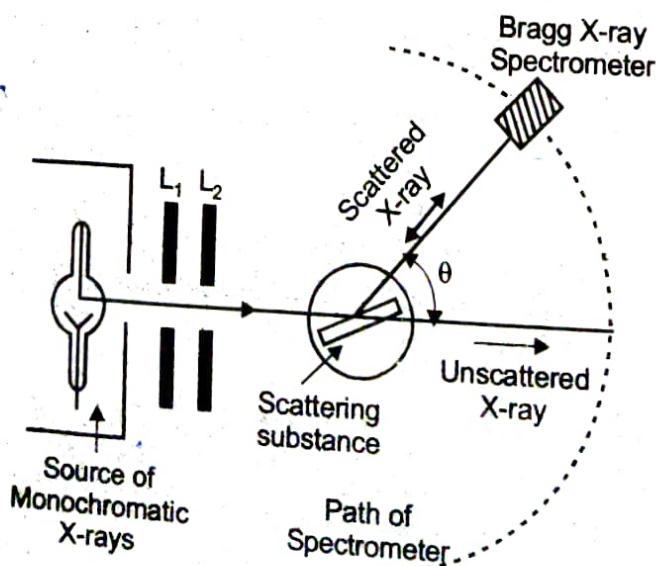
When  $\theta = 180^\circ$ ,  $\cos \theta = -1$ , then

$$d\lambda = \frac{2h}{m_e c} = \frac{2 \times 6.625 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} = 0.0485 \text{ Å}$$

The change in wavelength is maximum at the scattering angle of  $\theta = 180^\circ$ .

### 4.3.2 Experimental Verification

A beam of monochromatic X-rays of wavelength  $\lambda$  is made to fall on a scattering material like a block of carbon as shown in Fig. 4.6. The spectrometer can freely swing in an arc about the scattering beam.



**Fig. 4.6: Experimental verification of Compton effect**

The wavelength and intensity of the scattered X-rays received by the spectrometer is measured for various values of the scattering angles. Graphs are plotted between the intensity of the scattered X-rays and wavelength for various scattering angles as shown in Fig. 4.7.

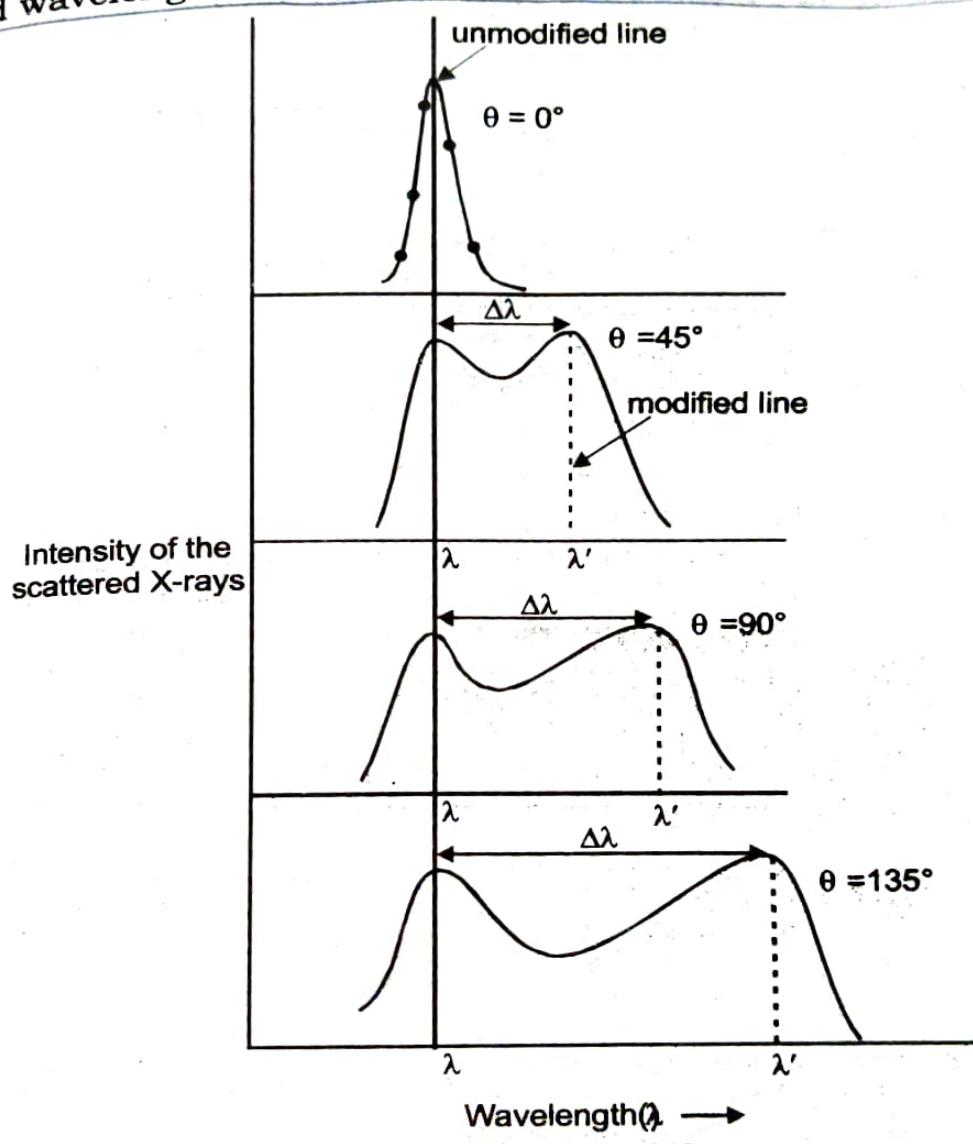


Fig. 4.7 : Compton shift

From the graphs, it is understood that in the scattered radiation, in addition to the incident wavelength ( $\lambda$ ) there exists a line of longer wavelength ( $\lambda'$ ). The Compton shift ( $d\lambda$ ) is found to vary with the scattering angle and the shift is greater for higher scattering angle.

The change in wavelength ( $d\lambda = 0.0243\text{Å}$ ) at  $\theta = 90^\circ$  is found to be in good agreement with the theoretical value. Thus Compton effect is experimentally verified and explains the corpuscular nature of radiation and the validity of quantum concept very well.

## SOLVED PROBLEMS

### PROBLEM 4.1

In a Compton scattering experiment the incident photons have wavelength of  $3 \times 10^{-10}$  m. Calculate the wavelength of scattered photons if they are viewed at an angle of  $60^\circ$  to the direction of incidence. (AU, April 2003)

**Solution:**

Incident wavelength  $\lambda = 3 \times 10^{-10}$  m and  $\theta = 60^\circ$

$$\begin{aligned}\lambda' - \lambda &= \frac{h}{m_e c} (1 - \cos \theta) \\ \lambda' &= \lambda + \frac{h}{m_e c} (1 - \cos \theta) \\ &= 3 \times 10^{-10} + \frac{6.626 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} (1 - \cos 60^\circ) \\ &= 3 \times 10^{-10} + 0.01232 \times 10^{-10} \\ &= 3.012 \times 10^{-10} \text{ m}\end{aligned}$$

The wavelength of scattered photon =  $3.012 \text{ \AA}$

### PROBLEM 4.2

Find the change in wavelength of an X-ray photon when it is scattered through an angle of  $90^\circ$  by a free electron. (AU, Jan 2004)

**Solution:**

Velocity of light ( $c$ ) =  $3 \times 10^8$  m/s

Mass of electron ( $m$ ) =  $9.1 \times 10^{-31}$  kg

Planck's constant ( $h$ ) =  $6.626 \times 10^{-34}$  joule second

Angle of scattering( $\theta$ ) =  $90^\circ$

$$\begin{aligned}\text{The change in wavelength } d\lambda &= \frac{h}{m_e c} (1 - \cos \theta) \\ &= \frac{6.626 \times 10^{-34} (1 - \cos 90^\circ)}{9.1 \times 10^{-31} \times 3 \times 10^8}\end{aligned}$$

The change in wavelength  $d\lambda = 2.42 \times 10^{-12}$  m

## 4.4 WAVE PARTICLE DUALITY

In 1924 Louis de Broglie of France postulated that nature is symmetrical in many ways and the universe is made of radiation (light) and matter (particle).

Experimental results show that light behaves as particle based on photoelectric effect and Compton effect, but as waves based on interference and diffraction.

So, light radiation exhibits both particle and wave nature. Louis de Broglie suggested that an electron or any other material particle like proton must also exhibit the wave like properties when they are in motion. This property is known as **Particle duality**. The waves associated with these material particles are known as **matter waves** or **de Broglie waves**.

### 4.4.1 Louis de Broglie Wavelength

Light has a dual nature namely particle nature as well as wave nature. So the energy of a photon can be written in two ways.

- Considering light as a wave of frequency  $\nu$ , the energy of the wave can be calculated according to Planck's hypothesis as  $E = h\nu$ .
- Considering light as a particle of mass  $m$  travelling with a velocity of  $c$ , the energy of the particle can be calculated according to Einstein mass-energy relation as  $E = mc^2$ .

Comparing these two equations we can write  $E = h\nu = mc^2$ .

$$\text{Now the momentum of the photon } p = mc = \frac{h\nu}{c} = \frac{h}{\lambda} \quad [\text{As } c = \lambda\nu]$$

Hence, the wavelength of a matter wave

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

Where  $m$  is the mass and  $v$  is the velocity of the particle. The above equation is known as Louis de Broglie's relation or matter wave equation. The waves associated with the moving material particles are called matter waves and using the above equation we can calculate the wavelength associated with the material particles.

This equation can be applied to all atomic particles like proton, neutron and electron. Davison and Germer experiment and G.P.Thomson experiment using electrons as incident beam proved the wave nature of the material particles and confirmed de Broglie's hypothesis of matter waves.

#### 4.4.2 de Broglie Wavelength Associated with Moving Electrons

Let us consider an electron traveling with a kinetic energy  $\frac{1}{2} mv^2$  under the influence of an electric field of potential difference  $V$  volts, where  $m$  is the mass of electron and  $v$  is the velocity. The energy of electron is  $eV$  where  $e$  is the charge of electron.

$$\text{Therefore, } \frac{1}{2} mv^2 = eV$$

$$mv^2 = 2eV$$

$$m^2v^2 = 2meV$$

$$mv = \sqrt{2meV}$$

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

$$= \frac{h}{\sqrt{2meV}}$$

$$= \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times V}}$$

Simplifying the equation we get,

$$\boxed{\lambda = \sqrt{\frac{150}{V}} \text{ Å}}$$

From the above equation we can calculate the wavelength of the electron moving under the influence of a potential difference of  $V$  volts.

### 4.4.3 Properties of Matter Waves

- Any 4*
- i) A material particle will have a matter wave just as a light quantum has a light wave.
  - ii) The wavelength of matter waves is given by  $\lambda = \frac{h}{p} = \frac{h}{mv}$ , where m is the mass and v is the velocity of the particle.
  - iii) If m is large or v is large, the wavelength associated with the particle is small.
  - iv) The matter waves are thus generated when the particles are in motion.
  - v) The wavelength associated with a particle is independent of any charge associated with it. (as there is no charge term in the equation for  $\lambda$ )
  - vi) The confirmation of matter wave assign dual nature to the particle.
  - vii) Matter waves are not electromagnetic waves. They are different type of waves.

We know that

$$E = hv = mc^2$$

Hence  $v = \frac{mc^2}{h}$

Therefore, the velocity of the matter wave

$$v_w = v\lambda = \frac{mc^2}{h} \cdot \frac{h}{mv_p}$$

Where,  $v_p$  = Velocity of the particle

$$\therefore v_w = \frac{c^2}{v_p}$$

As  $v_p$  is always less than 'c' the velocity of light,  $v_w \gg c$ .

- viii) In a single experiment or phenomenon, both particle and wave nature do not occur simultaneously.

## SOLVED PROBLEMS

### PROBLEM 4.3

An electron is accelerated by a potential difference of 150 V. What is the wavelength of the electron wave?  
 (AU, Dec 2004)

**Solution:**

$$\text{Accelerated voltage of electron} = 150 \text{ V}$$

The wavelength of de Broglie wavelength for an electron wave

$$\begin{aligned}\lambda &= \sqrt{\frac{150}{V}} = \sqrt{\frac{150}{150}} \\ &= 1 \text{ \AA}\end{aligned}$$

### PROBLEM 4.4

Calculate the de Broglie wavelength associated with a proton moving with a velocity equal to one thirtieth of the velocity of light.  
 (AU, Dec 2003)

**Solution:**

$$\begin{aligned}\text{Velocity of proton } (v) &= \text{Velocity of light} \times \frac{1}{30} \\ &= \frac{1}{30} \times 3 \times 10^8 \\ &= 1 \times 10^7 \text{ m/s}\end{aligned}$$

$$\text{Mass of proton } (m) = 1.67 \times 10^{-27} \text{ kg}$$

$$\text{Planck's constant } (h) = 6.625 \times 10^{-34} \text{ joule second}$$

$$\begin{aligned}\text{de Broglie wavelength } \lambda &= \frac{h}{mv} \\ &= \frac{6.625 \times 10^{-34}}{9.1 \times 10^{-31} \times 1 \times 10^7} \\ &= 3.5612 \times 10^{-13} \text{ m}\end{aligned}$$

## QUANTUM PHYSICS

## PROBLEM 4.5

Calculate the de Broglie wavelength of an electron having velocity of  $10^6$  m/s.

*Solution:*

$$\text{Velocity of electron } (v) = 10^6 \text{ m/s}$$

$$\text{Mass of electron } (m) = 9.1 \times 10^{-31} \text{ kg}$$

$$\text{Planck's constant } (h) = 6.626 \times 10^{-34} \text{ joule second}$$

$$\begin{aligned}\text{de Broglie wavelength } \lambda &= \frac{h}{mv} \\ &= \frac{6.626 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^6} \\ &= 7.25 \times 10^{-10} \text{ m} \\ &= 7.25 \text{ Å}\end{aligned}$$

## PROBLEM 4.6

A bullet of mass 1 gm is traveling with a velocity of 400 m/s. Calculate the de Broglie wavelength. (AU, Dec 2001)

*Solution:*

$$\text{Mass of the bullet } (m) = 1 \text{ gm} = 1 \times 10^{-3} \text{ kg}$$

$$\text{Velocity of the bullet } (v) = 400 \text{ m/s}$$

$$\text{Planck's constant } (h) = 6.626 \times 10^{-34} \text{ joule second}$$

$$\begin{aligned}\text{de Broglie wavelength } \lambda &= \frac{h}{mv} \\ &= \frac{6.626 \times 10^{-34}}{1 \times 10^{-3} \times 400} \\ &= 1.65 \times 10^{-33} \text{ m}\end{aligned}$$

**PROBLEM 4.7**

A neutron of mass  $1.675 \times 10^{-27}$  kg is moving with a kinetic energy 10 keV. Calculate the de Broglie wavelength associated with it. (AU, April 2003)

**Solution:**

$$\text{Kinetic energy } (E) = 10 \text{ keV}$$

$$= 10 \times 10^3 \times 1.6 \times 10^{-19} \text{ J}$$

$$\text{de Broglie wavelength } \lambda = \frac{h}{mv}$$

$$= \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 1.675 \times 10^{-27} \times 1.6 \times 10^{-19} \times 10 \times 10^3}}$$

$$\lambda = 2.8596 \times 10^{-13} \text{ m}$$

**PROBLEM 4.8**

An electron at rest is accelerated through a potential of 5000 V. Calculate the de Broglie wavelength of matter wave associated with it. (AU, April 2003)

**Solution:**

$$\text{de Broglie wavelength } \lambda = \sqrt{\frac{150}{V}}$$

$$= \sqrt{\frac{150}{5000}}$$

$$= 0.1735 \text{ Å}$$

### What is quantum physics?

Quantum physics is the study of the behaviour of matter and energy at the molecular, atomic, nuclear, and even smaller microscopic levels. We need quantum mechanics to explain the behaviour of electrons in atoms or solids or the behaviour of atoms in molecules. In the early 20<sup>th</sup> century, it was discovered that the laws that govern macroscopic objects do not function the same in such small realms.

### Who developed quantum mechanics?

The birth of quantum mechanics is attributed to Max Planck's 1900 paper on black body radiation.

Development of the field was done by Max Planck, Albert Einstein, Niels Bohr, Werner Heisenberg, Erwin Schrödinger, and many others. Ironically, Albert Einstein had serious theoretical issues with quantum mechanics and tried for many years to disprove or modify it.

### How quantum mechanics differs from classical mechanics?

Classical mechanics is completely definite theory in the sense that the computational procedures do not introduce any statistical uncertainties into the system themselves. Quantum mechanics on the other hand is fundamentally a probabilistic theory.

### What's special about quantum physics?

Light waves act like particles and particles act like waves (called wave particle duality). Matter can go from one spot to another without moving through the intervening space (called quantum tunnelling). Information moves instantly across vast distances.

In fact, in quantum mechanics we discover that the entire universe is actually a series of probabilities. Fortunately, it breaks down when dealing with large objects, as demonstrated by the Schroedinger's Cat thought experiment.

## 4.6 SCHRÖDINGER WAVE EQUATION

De Broglie's idea of matter waves was developed into a rigorous mathematical theory by Schrödinger in 1926.

The essential feature here is the incorporation of the expression for De Broglie wavelength into the general classical wave equation. Using this the wave equation for a moving particle is derived which is known as Schrödinger's fundamental wave equation.

### 4.6.1 Time Independent Schrödinger Wave Equation (TISE)

According to De Broglie, a particle of mass ' $m$ ' moving with a velocity ' $v$ ' has associated with it a wave system of some kind of wavelength  $\lambda = \frac{h}{mv}$ . Through we have no knowledge of what vibrates, we can denote it by  $\psi$ , periodic changes in which are responsible for the wave system.

Now let us suppose that a system of stationary waves is associated to the particle. Referring the particle to the cartesian coordinate system, at any point  $x, y, z$  in the immediate vicinity of the particle,  $\psi$  undergoes periodic changes and its value at any instant 't' can be written as

$$\psi(x, y, z, t) = \psi_0(x, y, z) e^{-i\omega t} \quad .. (1)$$

Where  $\psi_0(x, y, z)$  is a function of  $x, y, z$  and gives the amplitude at the point considered.

$$\text{The angular frequency of the wave} = \omega = \left( \frac{2\pi}{\lambda} \right) v_{\omega}$$

Where ' $v_{\omega}$ ' is the velocity of the particle wave and  $\lambda$  is the DeBroglie wavelength.

$$\text{Hence, } \boxed{\psi(\vec{r}, t) = \psi_0(\vec{r}) e^{-i\omega t}} \quad .. (2)$$

The classical differential equation of the system can be written as,

$$\left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) = \frac{1}{v_{\omega}^2} \frac{\partial^2 \psi}{\partial t^2} \quad .. (3)$$

Where,  $\psi$  represents the wave displacement at time  $t$ .  $x, y, z$  are co-ordinates of the particle and  $v_o$  is the wave velocity. The equation can be rewritten as

$$\nabla^2 \psi = \frac{1}{v_o^2} \frac{\partial^2 \psi}{\partial t^2} \quad \dots (4)$$

Where,  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$  is called Laplacian operator.

Differentiating equation (2) twice with respect to time  $t$  we have,

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

$$\frac{\partial^2 \psi}{\partial t^2} = (-i\omega)(-i\omega) \psi_o e^{-i\omega t} = -\omega^2 \psi$$

Substituting the above equation in equation (4) we have

$$\nabla^2 \psi = -\frac{\omega^2}{v_o^2} \psi$$

$$\nabla^2 \psi + \frac{\omega^2}{v_o^2} \psi = 0 \quad \dots (5)$$

$$\text{We know that } \omega = 2\pi v = \frac{2\pi v_o}{\lambda}$$

$$\text{Hence } \frac{\omega}{v_o} = \frac{2\pi}{\lambda} \quad \text{or} \quad \frac{\omega^2}{v_o^2} = \frac{4\pi^2}{\lambda^2}$$

Substituting the value of  $\frac{\omega^2}{v_o^2}$  in equation (5) we have

$$\nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi = 0 \quad \dots (6)$$

$$\text{But we know } \lambda = \frac{h}{mv_p} \text{ or } \lambda^2 = \frac{h^2}{m^2 v_p^2}$$

(Here  $v_p$  = velocity of the particle)

Substituting the value of  $\lambda^2$  in equation (6) we can write

$$\nabla^2\psi + \frac{4\pi^2}{h^2}m^2v_p^2\psi = 0 \quad .. (7)$$

If  $E$  is the total energy of the particle,  $V$  is the potential energy and  $\frac{1}{2}mv_p^2$  is the kinetic energy, then

$$E = PE + KE$$

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

$$E - V = \frac{1}{2}mv_p^2$$

$$mv_p^2 = 2(E - V)$$

$$m^2v_p^2 = 2m(E - V) \quad .. (8)$$

Substituting equation (8) in equation (7)

$$\nabla^2\psi + \frac{4\pi^2}{h^2} \times 2m(E - V)\psi = 0$$

$$\boxed{\nabla^2\psi + \frac{4\pi^2}{h^2} \times 2m(E - V)\psi = 0} \quad .. (9)$$

From equation (9)  $\nabla^2\psi + \frac{2m}{h^2/4\pi^2}(E - V)\psi = 0$

By taking  $\hbar = \frac{h}{2\pi}$  we can rewrite the above equation

$$\boxed{\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0} \quad \text{or} \quad \boxed{\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi} \quad .. (10)$$

This equation is known as the three-dimensional Schrödinger's time independent wave equation.

If we consider one dimensional motion, that is, particle moving along only in  $x$ -direction, the Schrodinger time independent equation reduces to

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad \dots (11)$$

For a free particle  $V = 0$ , the above equation is reduced to the following form

$$\nabla^2\psi + \frac{2m}{\hbar^2} E\psi = 0 \quad \dots (12)$$

This equation is known as the three-dimensional Schrödinger's wave equation for free particle.

#### 4.6.2 Time Dependent Schrödinger Wave Equation (TDSE)

Schrodinger time dependent wave equation is derived from Schrodinger time independent wave equation. The solution of classical differential equation of wave motion is given by,

$$\psi = \psi_0 e^{-i\omega t} \quad \dots (1)$$

Differentiating equation (1) with respect to time  $t$ , we get

$$\begin{aligned} \frac{\partial\psi}{\partial t} &= -i\omega\psi_0 e^{-i\omega t} \\ &= -i2\pi\nu\psi_0 e^{-i\omega t}, \quad \text{since } \omega = 2\pi\nu \end{aligned}$$

$$\frac{\partial\psi}{\partial t} = -i2\pi \frac{E}{\hbar} \psi, \quad \text{since } \nu = \frac{E}{\hbar}$$

$$\frac{\partial\psi}{\partial t} = \frac{-iE}{\hbar/2\pi} \psi$$

$$\frac{\partial\psi}{\partial t} = \frac{-iE}{\hbar} \psi, \quad \text{since } \hbar = \frac{\hbar}{2\pi}$$

Multiplying  $i$  on both sides,

$$i \frac{\partial \psi}{\partial t} = \frac{-i^2 E}{\hbar} \psi$$

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

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

.. (2)

Substituting the value of  $E\psi$  in equation  $\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$

$$\nabla^2 \psi + \frac{2m}{\hbar^2} \left( i\hbar \frac{\partial}{\partial t} - V \right) \psi = 0$$

$$\nabla^2 \psi = \frac{-2m}{\hbar^2} \left( i\hbar \frac{\partial}{\partial t} - V \right) \psi$$

Multiplying throughout by  $\frac{-\hbar^2}{2m}$

$$\frac{-\hbar^2}{2m} \nabla^2 \psi = i\hbar \frac{\partial \psi}{\partial t} - V\psi$$

$$\boxed{\frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \frac{\partial \psi}{\partial t}} \quad .. (2)$$

Where  $\psi$  is the wave function,  $E$  is the total energy and  $V$  is the potential energy of the particle. The above equation is the time dependent Schrödinger wave equation.

Equation (2) may be rewritten as

$$\left[ \frac{-\hbar^2}{2m} \nabla^2 + V \right] \psi = i\hbar \frac{\partial \psi}{\partial t} \quad .. (3)$$

or

$$\boxed{H\psi = E\psi} \quad .. (4)$$

Where  $H = \left[ \frac{-\hbar^2}{2m} \nabla^2 + V \right]$  is the Hamiltonian operator and

$E = i\hbar \frac{\partial}{\partial t}$  is the energy operator.

### 4.6.3 Physical Significance of Wave Function $\psi$

- i) The variable quantity that characterizes the matter wave is called wave function  $\psi$ .
- ii) The wave function connects the particle and wave nature statistically.
- iii) The wave function  $\psi$  is a variable quantity that is associated with a moving particle at any position  $(x, y, z)$  and at any time  $t$  and it relates the probability of finding the particle at that point and at that time.
- iv) The wave function  $\psi$  can give the probability amplitude of the position of the particle at a time but it cannot predict the exact location of the particle at that time.
- v) The wave function  $\psi$  is a complex quantity and it does not have any physical meaning by itself, but when we multiply this with its complex conjugate, the product  $\psi^* \psi = |\psi|^2$  has a physical meaning. This concept is similar to light. In light, the amplitude may be positive or negative but the intensity that is the square of amplitude is real and measurable.
- vi) The probability of finding the particle in a particular volume  $d\tau$  is given by  $\iiint \psi^* \psi d\tau = \iiint |\psi|^2 d\tau$ , where  $d\tau = dx dy dz$  and  $\psi^*$  is the complex conjugate of  $\psi$ .
- vii) If  $\iiint \psi^* \psi d\tau = 1$  then the particle is certainly present and if  $\iiint \psi^* \psi d\tau = 0$ , then the particle is not present.
- viii) The probability density is given by the equation  $P(\bar{r}, t) = |\psi(\bar{r}, t)|^2 = \psi^* \psi$

### 4.7 PARTICLE IN ONE-DIMENSIONAL BOX

Let us consider a potential well with finite width  $a$  and infinite depth in which an electron is placed (Fig. 4.9). We assume that the movement of the electron is restricted by the sides of the walls and the electron is moving only in the X-direction. When the electron collides with the walls, there is no loss of energy and so the collision considered to be perfectly elastic.

Since the electron is moving freely inside the potential well, its potential energy  $V = 0$ . But the potential energy of the electron is infinity on both sides of the well and outside the well. The wall of potential well acts as a potential barrier, which protects the electron, inside the potential well.

The potential outside the well is infinity. So the probability of finding the particle outside the well is zero.

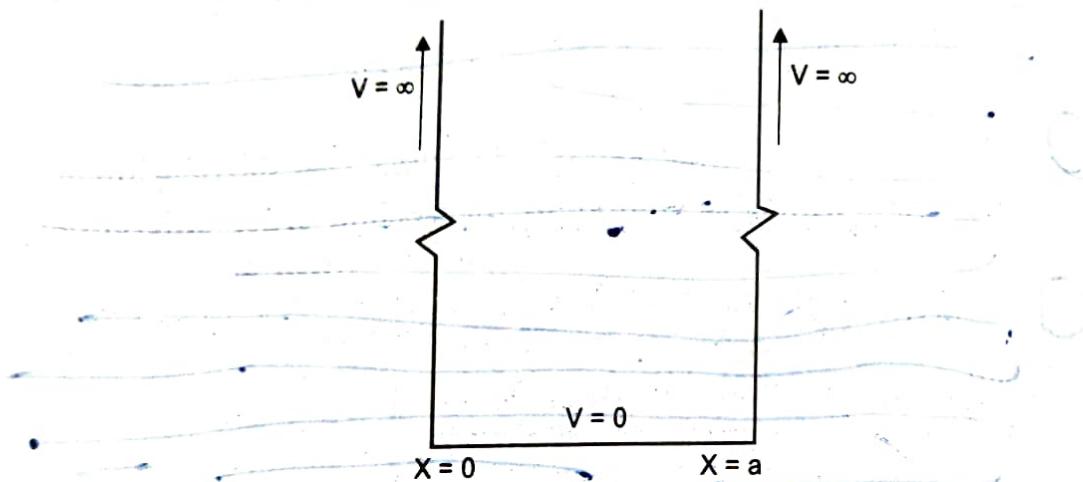


Fig. 4.9: One-dimensional potential well

That is,  $V = \infty$  and  $|\psi|^2 = 0$  for  $0 \geq x \geq a$

Therefore,  $\psi = 0$  at  $x \leq 0$  and  $x \geq a$

The potential inside the well is zero. So the probability of finding the particle inside the well is not zero.

That is,  $V = 0$  and  $|\psi|^2 \neq 0$  for  $0 < x < a$

Therefore,  $\psi \neq 0$  at  $x > 0$  and  $x < a$

The one dimensional Schrödinger wave equation is written as

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

When the electron is inside the potential well, the potential energy  $V = 0$  and  $E$  is completely equal to the kinetic energy of the electron. Thus, the equation reduces to the form,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi(x) = 0 \text{ since } V = 0 \quad \dots (2)$$

*KL*

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

Where,  $k^2 = \frac{2mE}{\hbar^2} = \frac{2m}{\hbar^2} \times \frac{p^2}{2m}$  since  $E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m}$

$$k^2 = \frac{p^2}{\hbar^2} = \frac{4\pi^2 p^2}{h^2} = \frac{4\pi^2}{\lambda^2} \text{ since } \lambda = \frac{h}{p} \text{ or } \frac{p^2}{h^2} = \frac{1}{\lambda^2}$$

Therefore,  $k = \frac{2\pi}{\lambda}$  is called the wave vector or wave number.

Equation (2) is the wave equation for the free particle inside the potential well, which is similar to the second order differential equation. The solution of the equation can be written as

$$\psi(x) = A \sin kx + B \cos kx \quad .. (3)$$

To evaluate the constants  $A$  and  $B$  let us apply the boundary conditions.

$$\psi = 0 \text{ at } x = 0 \text{ and } x = a$$

$$\text{When } x = 0, \psi(x) = 0$$

With the above condition  $B$  must be zero

$$\text{When } x = a, \psi(x) = 0$$

$$A \sin ka = 0$$

Since  $A$  is not equal to zero,  $\sin ka = 0$  and hence,  $ka = n\pi$  where  $n = 1, 2, 3, \dots$

$$\text{or } k = \frac{n\pi}{a} \quad .. (4)$$

We know,

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

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2\hbar^2}{8ma^2}$$

$$\text{since } \hbar^2 = \frac{h^2}{4\pi^2} \quad .. (5)$$

*Velocity*

Based on equation (5) the energy values of electrons are discrete so that electron will be in any one of the above energy states or eigen states at a given time.

These energy values are often referred to as eigen values or allowed values and occur in all quantum mechanical problems concerning spatially bound or constrained particles. The number  $n$  is called as a quantum number. The lowest eigen state is called ground state.

$$\text{When } n = 1, \text{ the lowest energy level } E_1 = \frac{\hbar^2}{8ma^2}$$

with  $k = \frac{n\pi}{a}$  and  $B = 0$ , equation (3) can be rewritten as as

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{a}\right) \quad \dots (6)$$

The value of  $A$  can be evaluated by applying normalization condition.

The probability of finding the particle inside the potential well of width  $a$  is unity. It can be written as

$$\int_0^a |\psi_n(x)|^2 dx = 1$$

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

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

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

$$\frac{A^2}{2} a = 1 \text{ or } A = \sqrt{\frac{2}{a}}$$

The normalization wave function can be written as

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)} \quad \dots (7)$$

function

The wave function  $\psi_n$  and the corresponding energies  $E_n$  are called as eigen functions and eigen values respectively describing the quantum state of the particle. The first three electron energy levels and their corresponding wave function and probability densities are illustrated in Fig. 4.10.

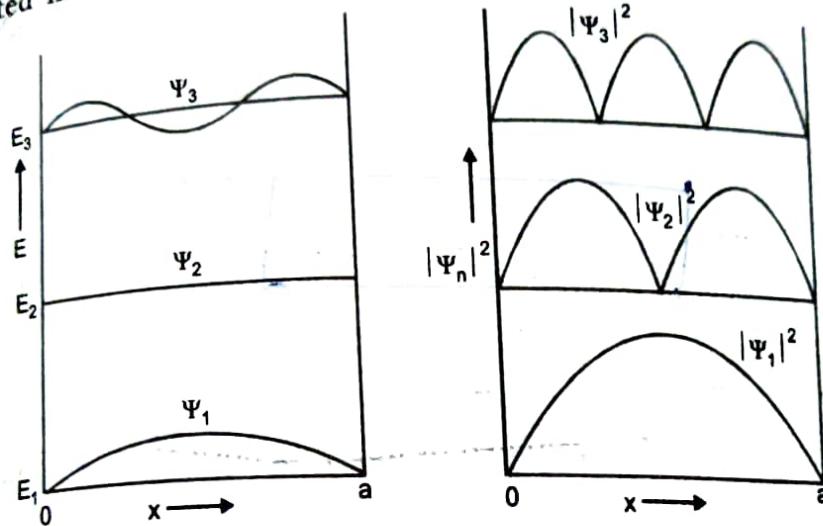


Fig. 4.10: The first three electron energy levels and probability densities

We thus find that the electrons can have only discrete energy levels and that the electrons will be in any one of the eigen states  $\psi_n$  at a given time.

For a value of  $L = 1 \text{ \AA}$  (Microscopic value)

$$E_n = \frac{n^2 (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times 10^{-20}} \text{ J}$$

$$E_n = 38 n^2 \text{ eV}$$

$$E_1 = 38 \text{ eV}; E_2 = 152 \text{ eV}; E_3 = 342 \text{ eV} \text{ etc.}$$

Note that the levels are quite far apart.

If  $L = 1 \text{ cm}$  (i.e., for Macroscopic dimension)

$$E_n = 38 \times 10^{-16} n^2 \text{ eV}$$

$$\therefore E_1 = 38 \times 10^{-16} \text{ eV}; E_2 = 152 \times 10^{-16} \text{ eV}; E_3 = 342 \times 10^{-16} \text{ eV etc.}$$

Hence the energy levels are very close to each other and appear to be continuous.

Also from the graph (Figure 2), it is clear that the probability of finding the electrons in state  $\psi_1$  (i.e., energy  $E_1$ ) is maximum at the centre of the box and the probability of finding the electrons in state  $\psi_2$  (energy  $E_2$ ) is **zero** at the centre of the box.

### Particle in a 3D box (electrons in a metal)

The solution for the 1D potential well can be extended to 3D (realistic situation).

With a cubical box of length  $L$ ,

$$E_n = \frac{\hbar^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$

where  $n_x, n_y, n_z$  can take values 1, 2, 3, ...

and

$$\psi_n = \sqrt{\frac{8}{L^3}} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)$$

$$\text{Here } n^2 = n_x^2 + n_y^2 + n_z^2$$

From the above, it is clear that

1. Three integers  $n_x, n_y, n_z$  called **quantum numbers** are required to completely specify an energy state.  
Since the particle exists in the box, none of the quantum numbers can be zero. (As  $\psi \neq 0$ ). The minimum value would be (111).
2.  $E$  depends on the sum of squares of the quantum numbers and not on the individual values.
3. Several combinations of the 3 quantum numbers may give rise to different wave functions but same energy value. Such states are called **degenerate states**.

### Degeneracy

Different wave functions with 3 different quantum numbers may lead to same value of energy. This is referred to as **degeneracy**.

Example: 3 independent states having (112); (121) and (211) have the same energy as shown below.

$$E_{211, 112, 121} = \frac{6h^2}{8mL^2} \quad (\text{As } n_x^2 + n_y^2 + n_z^2 = 2^2 + 1^2 + 1^2 = 6)$$

These levels are **triply degenerate** or **3-fold degenerate**.

(111); (222) etc are **non-degenerate**

i.e.,  $\Psi_{111}$ ;  $\Psi_{222}$  are non-degenerate  
and  $\Psi_{211}$ ,  $\Psi_{121}$ ,  $\Psi_{112}$  are degenerate.

Degeneracy can be broken by application of a magnetic field or electric field to the system.

### Electrons in a metal

Consider a metal piece of cubic cm dimension (i.e., a 3D box with  $L = 1$  cm (Macroscopic))

For ground state energy  $n_x = n_y = n_z = 1$

$$\text{i.e., } E_{111} = \frac{h^2}{8mL^2} (1^2 + 1^2 + 1^2)$$

$$E_{111} = \frac{3h^2}{8mL^2}$$

$$E_{111} = 1.806 \times 10^{-33} \text{ J}$$

$$E_{111} = 1.129 \times 10^{-14} \text{ eV}$$

To calculate separation between consecutive energy levels consider the next level after ground state i.e., (211)

$$E_{211} = \frac{h^2}{8mL^2} (2^2 + 1^2 + 1^2) = \frac{6h^2}{8mL^2}$$

$$E_{211} = 2.258 \times 10^{-14} \text{ eV}$$

We see that the separation between consecutive levels is of the order of  $10^{-14}$  eV. Energy of the ground state is around  $10^{-14}$  eV and can be considered zero. As consecutive levels are separated by a small value, the energy distribution can be regarded as **quasi-continuous**.

The above results indicate that even the pool of free electrons (electrons gas) have quantised energies and thus have a distribution of energies and do not possess the same average energy as indicated in classical theory.

**SOLVED PROBLEMS****PROBLEM 4.9**

Give the lowest energy value of a particle of mass  $m$  trapped in a one-dimensional potential box of length  $a$ .  
 (AU, April 2002)

**Solution:**

$$\text{The energy eigen values } E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$= \frac{n^2 \hbar^2}{8ma^2}$$

The energy is lowest when  $n = 1$

$$\text{The lowest energy value } E_l = \frac{\hbar^2}{8ma^2}$$

**PROBLEM 4.10**

Calculate the lowest energy level of an electron confined in a well of 1 Å width.  
 (AU, Jan 2007)

**Solution:**

$$\text{Plank's constant } (h) = 6.625 \times 10^{-34} \text{ joule second}$$

$$\text{Mass of electron } (m) = 9.1 \times 10^{-31} \text{ kg}$$

$$\text{Width of the potential well } (a) = 1 \times 10^{-10} \text{ m}$$

$$\text{Lowest energy level } n = 1$$

$$\text{The energy eigen values } E_n = \frac{n^2 \hbar^2}{8ma^2}$$

$$= \frac{1^2 \times (6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10^{-10})^2} \text{ J}$$

$$= \frac{1^2 \times (6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10^{-10})^2 \times 1.6 \times 10^{-19}} \text{ eV}$$

$$= 38 \text{ eV}$$

**PROBLEM 4.11**

An electron is trapped in a one-dimensional box of length 0.1 nm. Calculate the energy required to excite the electron from its ground state to the sixth excited state.

(A.U. April 2003)

**Solution:**

$$\text{Length } a = 0.1 \text{ nm}$$

$$= 0.1 \times 10^{-9} \text{ m}$$

$$\text{The energy eigen values } E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$= \frac{n^2 \hbar^2}{8ma^2}$$

For ground state  $n = 1$

$$\begin{aligned} \text{The energy value } E_1 &= \frac{1^2 \times (6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10^{-10})^2} \\ &= 0.0602 \times 10^{-16} \text{ J} \end{aligned}$$

For 6<sup>th</sup> excited state  $n = 7$

$$\begin{aligned} \text{The energy value } E_7 &= \frac{7^2 \times (6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10^{-10})^2} \\ &= 2.1680 \times 10^{-16} \text{ J} \end{aligned}$$

The energy required to excite the electron from its ground state to the sixth excited state is  $E = E_7 - E_1$

$$\begin{aligned} \text{The energy required} &= 2.1680 \times 10^{-16} - 0.0602 \times 10^{-16} \\ &= 2.1078 \times 10^{-16} \text{ J} \\ &= \frac{2.1078 \times 10^{-6}}{1.6 \times 10^{-19}} \text{ eV} \\ &= 1.317 \times 10^3 \text{ eV} = 1.3170 \text{ KeV} \end{aligned}$$

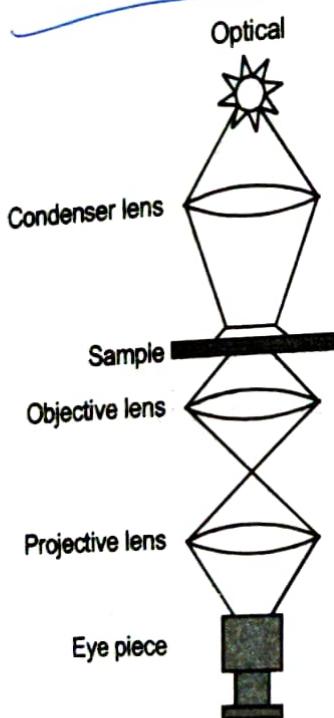
4.44

## 4.8 INTRODUCTION TO MICROSCOPE

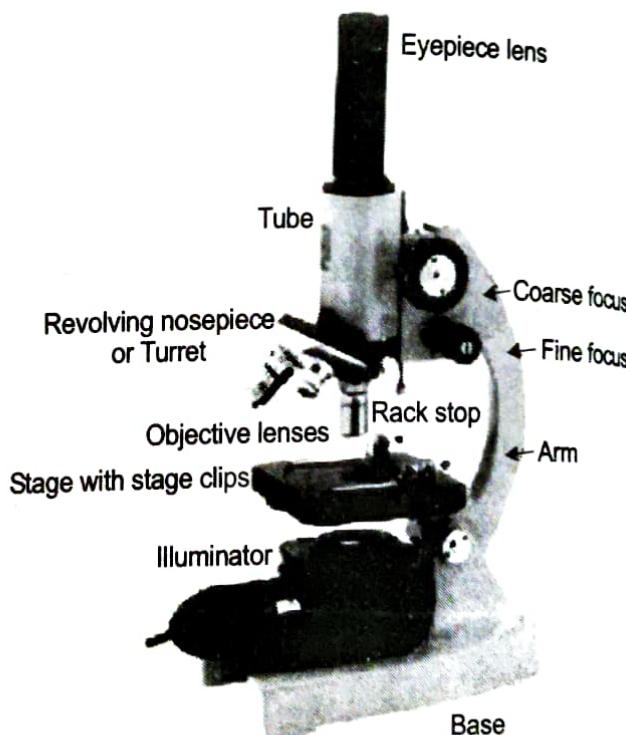
Before we can understand how the optical and electron microscope work, it is important that we distinguish between **resolution** and **magnification**. Magnification is how much bigger we can make something appear. Resolution is how much better we can distinguish two closely spaced points.

### 4.8.1 Optical Microscope

It is an optical tool which gives rise to higher magnification and resolution images of an object and is shown in Fig. 4.11.



(a)



(b)

Fig. 4.11

### 1. Limitations of Optical Microscopy

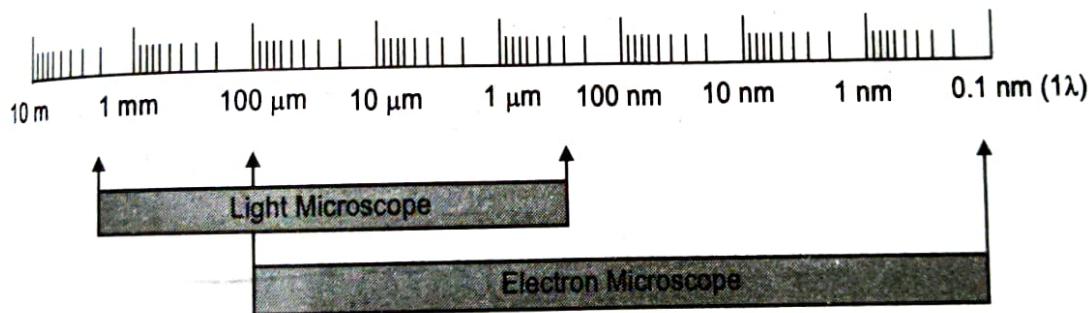
- i) The resolution  $R$  depends on the angular aperture  $\alpha$ :

$$R = \frac{1.22 \lambda}{2 \times \text{N.A.}} = \frac{1.22 \lambda}{2n \sin \theta}$$

Here  $\theta$  is the collecting angle of the lens, which depends on the width of objective lens and its focal distance from the specimen.  $n$  is the refractive index of the medium in which the lens operates.  $\lambda$  is the wavelength of light illuminating or emanating from (in the case of fluorescence microscopy) the sample. The quantity  $n \sin\theta$  is also known as the numerical aperture (N.A.).

Due to the limitations of the values  $\theta$ ,  $\lambda$ , and  $n$ , the **resolution limit** of a light microscope using visible light is **about 200 nm**. This is because  $\theta$  for the best lens is about  $70^\circ$  ( $\sin \theta = 0.94$ ), the shortest wavelength of visible light is blue ( $\lambda = 450 \text{ nm}$ ), and the typical high resolution lenses are oil immersion lenses ( $n = 1.56$ ):

$$R = \frac{1.22 \times 450 \text{ nm}}{2 \times 1.56 \times 0.94} = 187 \text{ nm}$$



2. The possible magnification is about 1000X.
3. Depth of focus is the measure of the distance through which the object could be moved towards or away from the objective lens but still producing a sharply focused image. Since it is inversely proportional to NA and magnification of the objective, depth of focus decreases with increase in magnification.

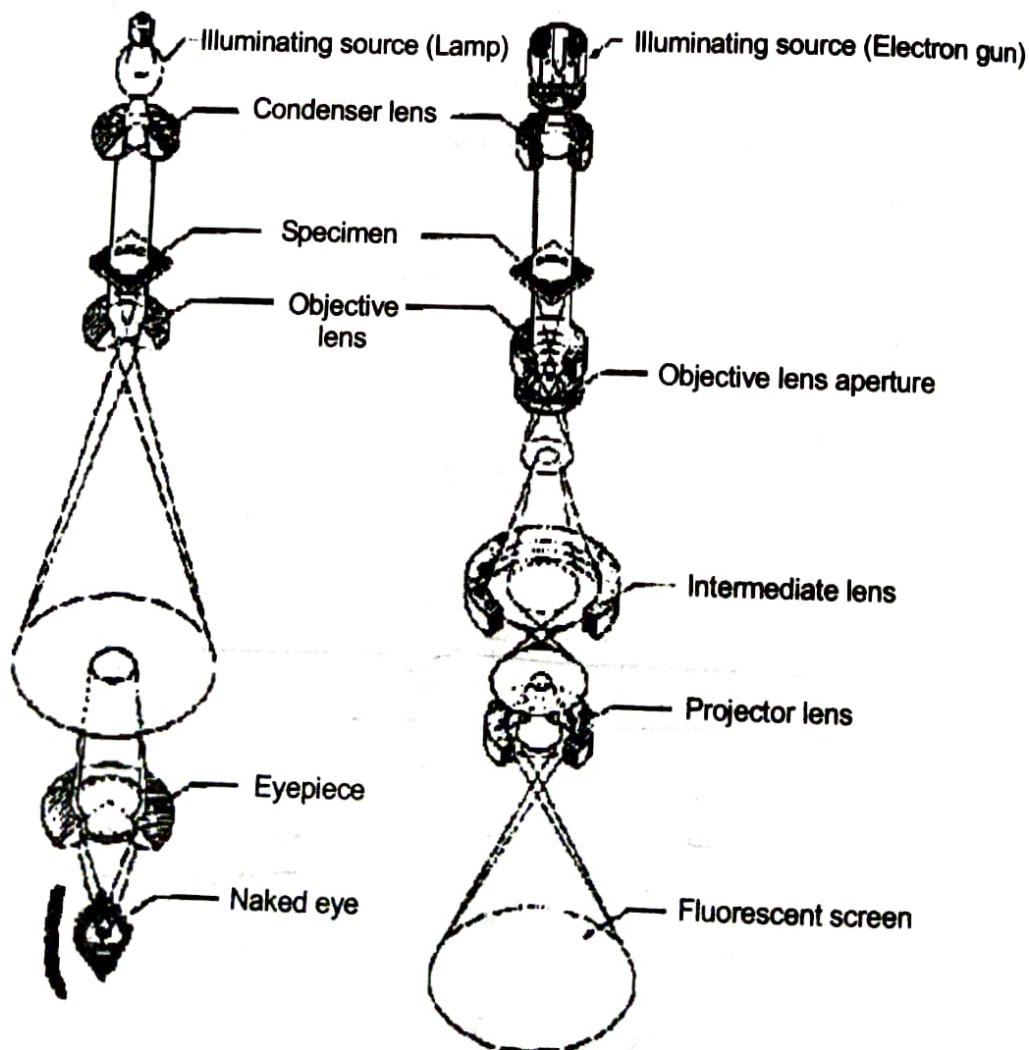
For example, depth of focus is 250 mm, for 15X magnification and 0.08 mm, for 1200X magnification

### 4.8.2 Electron Microscope

As one could not use visible light for higher resolution and magnification, it is clear that one has to use radiation of shorter wavelengths. Since the refractive index of glass is nearly unity at X-ray wavelength, X-ray too can not be used.

Since the accelerated electron beam behaves as waves at shorter wavelengths (higher frequencies), one can use electron beam for construction of a microscope.

For focusing the electron beam on a specimen, the current carrying coils producing magnetic fields are used. A comparison of optical and electron microscope is shown in Fig. 4.12 and Table 4.1.



(Optical microscope image)

(Electron microscope image)

Fig. 4.12

Table 4.1

	Optical microscope	Electron microscope
	Optical microscope	Electron microscope
Source	Optical light	Electron gun
Wavelength	7500 Å (visible) ~ 2000 Å (ultraviolet)	0.859 Å (20 kV) ~ 0.0370 Å (100 kV)
Lenses	Optical lenses	Electromagnetic lenses
Magnification	1,000X	10,00,000X
Resolution	200 nm	0.1 nm
Environment	Atmosphere	High vacuum

#### 4.8.3 Specimen Interactions

A schematic diagram of the various interactions in an electron microscope are shown in Fig. 4.13.

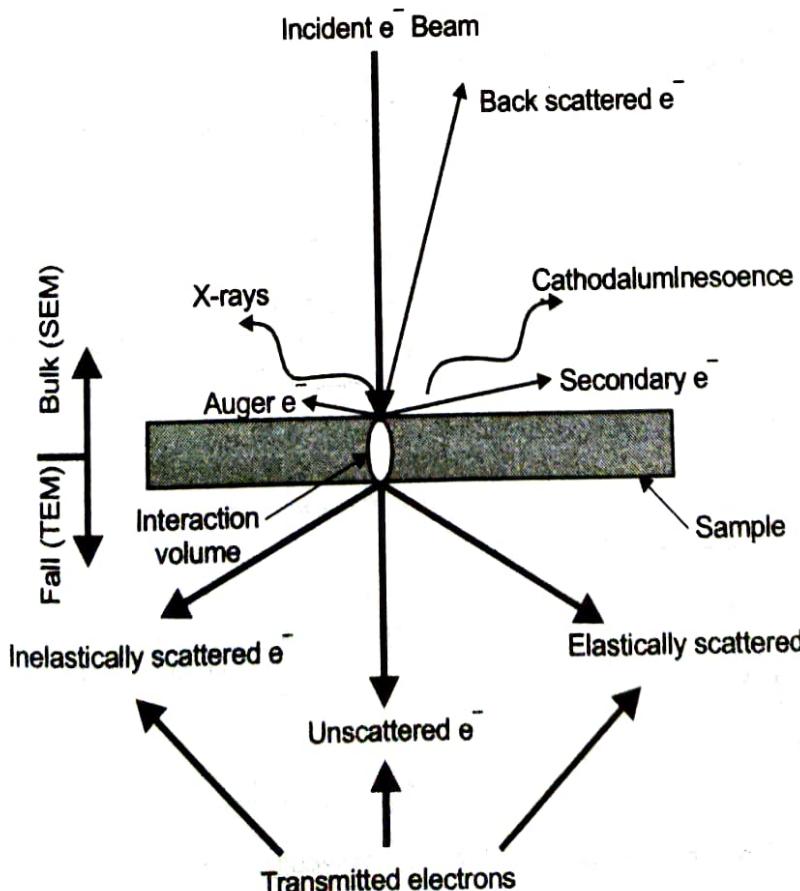


Fig. 4.13: Summary of the various output signals obtained by interaction of electrons with matter in an electron microscope

When the energetic electrons strike the sample, various interactions occur. The interactions occurring on the top side of the thick or bulk sample results in Scanning Electron Microscope (SEM), while the interactions occurring on the bottom side of the thin foil like sample result in Transmission Electron Microscope (TEM).

One can list the possible specimen interactions as follows:

### 1. Backscattered Electrons

- a) They are observed at nearly  $180^\circ$ .
- b) The intensity of scattered electrons depend on atomic number of specimen.
- c) The higher atomic number elements are brighter compared to lower atomic number electrons.
- d) Can be used to differentiate parts of the specimen that have different average atomic number.

### 2. Secondary Electrons

A beam of electrons moving nearer to the atom gives some energy to the K-shell electron. The ionized K-shell electrons with small K.E form the secondary electrons.

Since the energy of the secondary electrons is low, it is clear that the electrons from the surface only can be ejected and hence used in the topography (surface analysis).

### 3. Auger Electrons

Secondary electron can also be ejected from a core level leaving a vacancy.

An electron from a higher energy level may fall into the vacancy, resulting in a release of energy.

Although sometimes this energy is released in the form of an emitted photon (X-ray), the energy can also be transferred to another electron, which is ejected from the atom.

This second ejected electron is called an Auger electron, and is used for getting compositional information.

#### 4. X-Rays

Secondary electron is ejected from a core level leaving a vacancy. An electron from a higher energy level may fall into the vacancy, resulting in a release of energy. This energy is released in the form of an emitted photon (X-ray).

#### 5. Unscattered Electrons

Incident electrons which are transmitted through the thin specimen without any interaction occurring inside the specimen are called unscattered electrons.

Intensity of unscattered electrons vary inversely as the thickness of the specimen. Hence, thicker areas appear darker and thinner areas appear brighter.

#### 6. Elastically Scattered Electrons

These are the incident electrons that are scattered (deflected from their original path) by atoms in the specimen in an elastic fashion (no loss of energy).

These scattered electrons are then transmitted through the remaining portions of the specimen.

#### 7. Inelastically Scattered Electrons

They are the electrons that interact with specimen atoms in an inelastic fashion, losing energy during the interaction.

These electrons are then transmitted through the rest of the specimen.

#### 4.8.4 Scanning Electron Microscope (SEM) (Construction Working and Applications)

The basic construction of a SEM indicating the different parts is shown in Fig. 4.14.

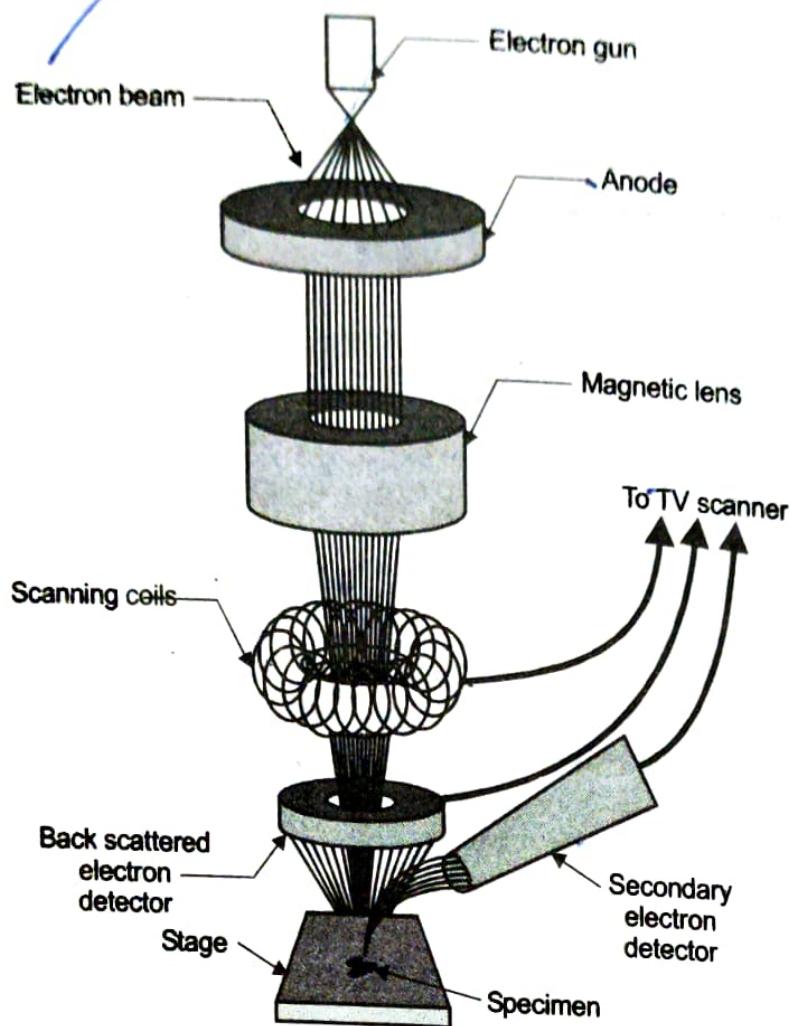


Fig. 4.14

#### 4.8.5 Anode, Magnetic Lens, Scanning Coils

- The Anode is used to eliminate high angle electrons
- The Magnetic Lens assists in getting a thin and coherent electron beam.
- The Scanning coils scan and sweep the beam in a grid fashion (as in TV). Hence the beam focusses and dwells on the desired point of the sample for some time.

#### Working

The image is produced by scanning the sample with a focussed electron beam and detecting the secondary and/or backscattered electrons. Electrons and photons are emitted from each and every point of the sample and observed using the detector.

**Applications**

SEM gives useful information on:

- 1. Topography:** The surface features of an object or "how it looks". Its texture, detectable features are limited to a few nanometers.
- 2. Morphology:** The shape, size and arrangement of particles making up the object that are lying on the surface of the sample or have been exposed by grinding or chemical etching. Detectable features limited to a few nanometers.
- 3. Composition:** The elements and compounds the sample is composed of and their relative ratios, in areas ~ 1 micrometer in diameter.
- 4. Crystallographic information:** The arrangement of atoms in the specimen and their degree of order. Only useful on single-crystal particles greater than 20 micrometers.

The most common use in the area of semi-conductor applications are,

1. To view the surface of the device.
2. For failure analysis.
3. Cross-sectional analysis to determine the device dimensions such as MOSFET channel length or junction depth.
4. On-line inspection of wafer processing production.
5. Inspection of integrated-circuits etc.

**4.8.6 Transmission Electron Microscope (TEM)**

Fig. 4.15 depicts the TEM.

**Working**

Clarification

The image is produced by observing the unscattered electrons, elastically and/or inelastically scattered electrons.

- **Condenser lens** is used to eliminate high angle electrons and make the beam coherent.
- **The Objective lens** focuses the beam into the image of specimen.
- **Projective lens** is used for further magnification of the image.

- Image is formed on the phosphor screen.
- The Darker areas are the thicker or denser sample areas.
- The Brighter areas are the thinner or less denser sample areas.

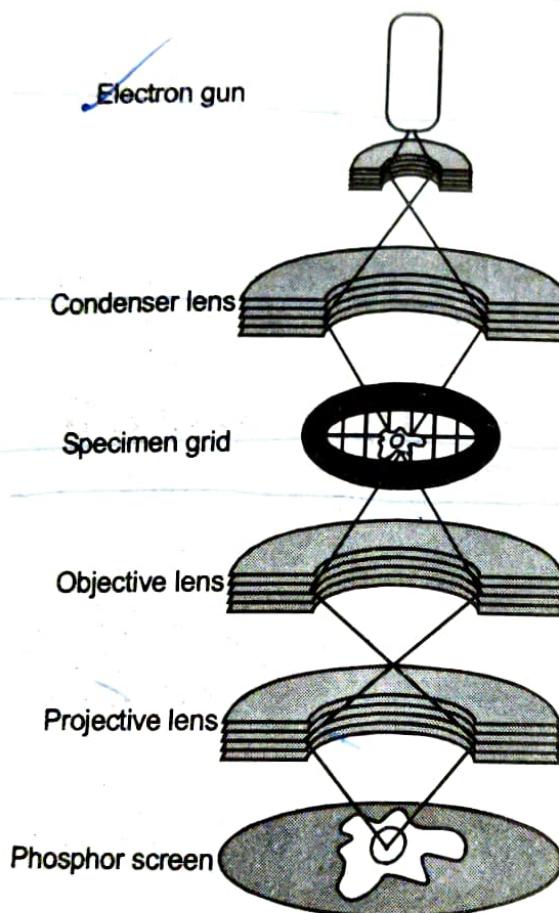


Fig. 4.15

### Applications

TEM gives the following useful information:

- Morphology:** The size, shape and arrangement of particles as well as their relationship to one another on the scale of atomic diameters.
- Crystallographic information:** The arrangement of atoms in the specimen and their degree of order, detection of atomic-scale defects a few nanometers in diameter.
- Compositional information:** The elements and compounds the sample is composed of and their relative ratios.

## SOLVED UNIVERSITY PROBLEMS

## PROBLEM 1

In Compton scattering, the incident photon has a wavelength 0.5 nm. Calculate the wavelength of scattered radiation if they are viewed at an angle of  $45^\circ$  to the direction of incidence. (AU, May 2009)

Given data:

$$\text{Wavelength of photon, } \lambda = 0.5 \text{ nm} = 0.5 \times 10^{-9} \text{ m}$$

$$\text{Angle of scattering } \theta = 45^\circ$$

Solution:

Wavelength of scattered X-ray

$$\lambda' = \lambda + \frac{h}{m_0 c} (1 - \cos \theta)$$

$$= 0.5 \times 10^{-9} + \frac{6.625 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} (1 - \cos 45)$$

$$= 0.5 \times 10^{-9} + 2.427 \times 10^{-12} \times (1 - 0.707)$$

$$= 0.5007 \times 10^{-9} \text{ m}$$

## PROBLEM 2

X-rays of photon of wavelength  $1.24 \times 10^{-3} \text{ Å}$  is scattered by a free electron through an angle of  $90^\circ$ . Calculate the energy of the scattered photon. (AU, Jan 2009)

Given data:

$$\text{Wavelength of incident photon, } \lambda = 1.24 \times 10^{-3} \text{ Å} = 1.24 \times 10^{-13} \text{ m}$$

$$\text{Angle of scattering } \theta = 90^\circ$$

Solution:

Wavelength of scattered X-ray

$$\lambda' = \lambda + \frac{h}{m_0 c} (1 - \cos \theta)$$

$$\begin{aligned}
 &= 1.24 \times 10^{-13} + \frac{6.625 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} (1 - \cos 90) \\
 &= 1.24 \times 10^{-13} + 2.4267 \times 10^{-12} \\
 &= 2.5507 \times 10^{-12} \text{ m}
 \end{aligned}$$

Energy of scattered photon

$$E = \frac{hc}{\lambda'} = \frac{6.625 \times 10^{-34} \times 3 \times 10^8}{2.5507 \times 10^{-12}}$$

$$= 7.7919 \times 10^{-14} \text{ J}$$

### PROBLEM 3

X-rays of wavelength  $1\text{\AA}$  are scattered from a carbon block. Calculate the Compton change in wavelength of the scattered beam scattered by an angle  $90^\circ$ .

(AU, May 2007)

Given data:

Wavelength of incident photon,  $\lambda = 1 \text{\AA} = 1 \times 10^{-10} \text{ m}$

Angle of scattering  $\theta = 90^\circ$

**Solution:**

Wavelength of scattered X-ray

$$\lambda' = \lambda + \frac{h}{m_0 c} (1 - \cos \theta)$$

$$\begin{aligned}
 &= 1 \times 10^{-10} + \frac{6.625 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} (1 - \cos 90) \\
 &= 0.0242 \times 10^{-10} \text{ m}
 \end{aligned}$$

**PROBLEM 4**

~~Calculate the equivalent wavelength of electron moving with a velocity of  $3 \times 10^7$  m/s.~~

(AU, Jan 2010)

Given data:

$$\text{Velocity of electron } v = 3 \times 10^7 \text{ m/s}$$

**Solution:**

$$\begin{aligned} \text{Wavelength of electron wave } \lambda &= \frac{h}{mv} = \frac{6.625 \times 10^{-34} \times 3 \times 10^8}{9.1 \times 10^{-31} \times 3 \times 10^7} \\ &= 2.4267 \times 10^{-11} \end{aligned}$$

**PROBLEM 5**

~~Calculate the de Broglie wavelength of an electron which has been accelerated from rest on application of potential of 400 volts.~~

(AU, Jan 2009)

Given data:

$$\text{Potential applied, } V = 400 \text{ volts}$$

**Solution:**

$$\begin{aligned} \text{Wavelength of electron wave } \lambda &= \frac{h}{\sqrt{2meV}} \\ &= \frac{12.26}{\sqrt{V}} \times 10^{-10} = \frac{12.26}{\sqrt{400}} \times 10^{-10} \\ &= 0.613 \times 10^{-10} \text{ m} \end{aligned}$$

**Alternate method:**

$$\text{Wavelength of electron wave } \lambda = \sqrt{\frac{150}{V}} = \sqrt{\frac{150}{400}} = 0.6123 \text{ Å}$$

**PROBLEM 6**

Calculate the de Broglie wavelength of an electron which has been accelerated from rest on application of potential of 100 volts.  
(AU, Jan 2011)

*Given data:*

$$\text{Potential applied, } V = 100 \text{ volts}$$

**Solution:**

$$\begin{aligned} \text{Wavelength of electron wave } \lambda &= \frac{h}{\sqrt{2meV}} = \frac{12.26}{\sqrt{V}} \times 10^{-10} \\ &= \frac{12.26}{\sqrt{100}} \times 10^{-10} = 1.226 \times 10^{-10} \text{ m} \end{aligned}$$

**Alternate method:**

$$\text{Wavelength of electron wave } \lambda = \sqrt{\frac{150}{V}} = \sqrt{\frac{150}{100}} = 1.226 \text{ Å}$$

**PROBLEM 7**

Calculate the de Broglie wavelength associated with a thermal neutron of energy 0.25 eV ( Mass of neutron =  $1.676 \times 10^{-27}$  kg, Planck's constant =  $6.625 \times 10^{-34}$  Js.

(AU, May 2004)

*Given data:*

$$\text{Energy of thermal neutron } E = 0.025 \text{ eV} = 0.025 \times 1.6 \times 10^{-19} \text{ J}$$

$$\text{Mass of neutron} \quad m = 1.67 \times 10^{-27} \text{ kg}$$

$$\text{Planck's constant,} \quad h = 6.625 \times 10^{-34} \text{ Js}$$

**Solution:**

Wavelength of neutron wave

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 0.025 \times 1.6 \times 10^{-19}}}$$

$$\text{Wavelength of neutron wave} = 1.8077 \times 10^{-15} \text{ m}$$

**PROBLEM 8**

Calculate the de Broglie wavelength of 10 keV neutron. Mass of neutron may be taken as  $1.675 \times 10^{-27}$  kg. (AU, May 2004)

Given data:

$$\text{Energy of thermal neutron } E = 10 \text{ keV} = 10 \times 10^3 \times 1.6 \times 10^{-19} \text{ J}$$

$$\text{Mass of neutron } m = 1.67 \times 10^{-27} \text{ kg}$$

$$\text{Planck's constant, } h = 6.625 \times 10^{-34} \text{ Js}$$

**Solution:**

$$\text{Wavelength of neutron wave } \lambda = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 10^4 \times 1.6 \times 10^{-19}}}$$

$$\text{Wavelength of neutron wave } \lambda = 2.861 \times 10^{-13} \text{ m}$$

**PROBLEM 9**

Find the lowest energy of the electron confined to move in a one dimensional box of length 1 Å. Given  $m_e = 9.1 \times 10^{-31}$  kg and  $h = 6.625 \times 10^{-34}$  Js. (AU, Jan 2008, 2014)

Given data:

$$\text{Length of one dimensional box } a = 1 \text{ Å} = 1 \times 10^{-10} \text{ m}$$

$$\text{Mass of electron } m_e = 9.1 \times 10^{-31} \text{ kg}$$

$$\text{Planck's constant } h = 6.625 \times 10^{-34} \text{ Js}$$

**Solution:**

The energy of electron confined in one dimensional box

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

For lowest energy  $n = 1$

Energy of lowest level

$$E_1 = \frac{h^2}{8ma^2} = \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (1 \times 10^{-10})^2}$$

$$= \frac{43.891 \times 10^{-68}}{72.8 \times 10^{-31} \times 1 \times 10^{-20}} = 0.6028 \times 10^{-17} \text{ J}$$

$$E_1 = 6.028 \times 10^{-18} \text{ J}$$

$$= 6.028 \times 10^{-18} \times \frac{1}{1.6 \times 10^{-19}} \text{ eV} = 37.675 \text{ eV}$$

### PROBLEM 10

An electron confined to a one dimensional box of side  $10^{-10}\text{m}$ . Obtain first two eigen values of the electron.

(AU, Jan 2010)

Given data:

Length of one dimensional box  $a = 1\text{\AA} = 1 \times 10^{-10} \text{ m}$

Mass of electron  $m_e = 9.1 \times 10^{-31} \text{ kg}$

Planck's constant  $h = 6.625 \times 10^{-34} \text{ Js}$

### Solution:

The energy of electron confined in one dimensional box

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

For lowest energy  $n = 1$

Energy of lowest level  $\text{J}$

$$E_1 = \frac{h^2}{8ma^2} = \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (1 \times 10^{-10})^2}$$

$$= \frac{43.891 \times 10^{-68}}{72.8 \times 10^{-31} \times 1 \times 10^{-20}} = 0.6028 \times 10^{-17} \text{ J}$$

$$E_1 = 6.028 \times 10^{-18} \text{ J}$$

$$= 6.028 \times 10^{-18} \times \frac{1}{1.6 \times 10^{-19}} \text{ eV} = 37.675 \text{ eV}$$

For the second energy level  $n = 2$

$$E_2 = \frac{n^2 h^2}{8ma^2} = \frac{4h^2}{8ma^2}$$

$$= 4E_1 = 37.68 \times 4 = 150.72 \text{ eV}$$

### PROBLEM 11

**Find the lowest energy of an electron confined in a box of length 0.2 nm.  
(AU, Dec 2010, Jan 2011)**

Given data:

$$\text{Length of one dimensional box } a = 0.2 \text{ nm} = 0.2 \times 10^{-9} \text{ m}$$

$$\text{Mass of electron } m_e = 9.1 \times 10^{-31} \text{ kg}$$

$$\text{Planck's constant } h = 6.625 \times 10^{-34} \text{ Js}$$

### Solution:

The energy of electron confined in one dimensional box

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

For lowest energy  $n = 1$

Energy of lowest level

$$E_1 = \frac{h^2}{8ma^2}$$

$$= \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (0.2 \times 10^{-9})^2}$$

$$= 1.507 \times 10^{-18} \text{ J}$$

$$E_1 = 1.507 \times 10^{-18} \text{ J}$$

$$= 1.507 \times 10^{-18} \times \frac{1}{1.6 \times 10^{-19}} \text{ eV}$$

$$= 9.4187 \text{ eV}$$

**PROBLEM 12**

~~An electron is confined between two walls 2.0 Å apart. Find the lowest energy possessed by the electron.~~

(AU, Dec 2007)

*Given data:*

Length of one dimensional box  $a = 2 \text{ \AA} = 2 \times 10^{-10} \text{ m}$

Mass of electron  $m_e = 9.1 \times 10^{-31} \text{ kg}$

Planck's constant  $h = 6.625 \times 10^{-34} \text{ Js}$

**Solution:**

The energy of electron confined in one dimensional box

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

For lowest energy  $n = 1$

Energy of lowest level

$$E_1 = \frac{h^2}{8 ma^2} = \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (2 \times 10^{-10})^2}$$

$$= \frac{4.3891 \times 10^{-67}}{2.912 \times 10^{-49}} = 1.5072 \times 10^{-18} \text{ J}$$

$$= 1.507 \times 10^{-18} \text{ J}$$

$$E_1 = 1.5072 \times 10^{-18} \times \frac{1}{1.6 \times 10^{-19}} \text{ eV} = 9.42 \text{ eV}$$

**SHORT QUESTIONS AND ANSWERS****PART - A****1. Define a black body.**

A perfect black body is defined as one, which completely absorbs radiations of all wavelengths incident on it and also emits radiations of all possible wavelengths when heated.

**2. What is black body radiation?**

A substance coated with lamp black may be considered a perfect black body for all practical purposes. The radiations emitted by a perfect black body are called black body radiations.

**3. What is Planck's hypothesis?**

(AU, Dec 2008)

Planck hypothesis are given as follows:

- i) The black body radiation chamber contains a large number of oscillating particles each vibrating with a characteristic frequency. These oscillations are called Planck oscillators.
- ii) The frequency of radiation emitted by an oscillator is the same as the frequency of its vibration.
- iii) The oscillator cannot absorb or emit energy in a continuous manner.
- iv) The oscillator can absorb or emit energy in the multiples of small unit called quantum. The quantum of radiation is called photon. The energy of a photon is  $h\nu$  where  $h$  is Planck's constant and  $\nu$  is the frequency.
- v) The oscillator vibrating with frequency can have only discrete energy values given by  $E = nh\nu$  where  $n = 1, 2, 3, \dots$ . The energy of the oscillator is thus quantized.
- vi) Planck's oscillators can emit or absorb radiation energy in packets of  $h\nu$ .

**4. Write Planck's radiation formula.**

(AU, Jan 2009)

The emission of energy per second per unit area per unit wavelength interval at wavelength  $\lambda$  is given by

$$E_\lambda = \frac{8\pi hc}{\lambda^5} \times \frac{1}{e^{\frac{h\nu}{kT}} - 1}$$

This is known as Planck's law of radiation formula.

**5. Write Wien's law derived from Planck's law.**

When  $\lambda$  is small and  $v$  is large, then  $e^{\frac{hv}{kT}} \gg 1$  and  $e^{\frac{hv}{kT}}$  is large compared to 1

$$\text{Then, } e^{\frac{hv}{kT}} - 1 = e^{\frac{hv}{kT}}$$

Then the Planck's law is reduced to

$$E_\lambda = \frac{8\pi hc}{\lambda^5 e^{\frac{hv}{kT}}}$$

This is known as Wien's law.

**6. Write Rayleigh Jean's law derived from Planck's law.**

When  $\lambda$  is longer and  $v$  is small, then  $e^{\frac{hv}{kT}} \gg 1$

$$\text{Then } e^{\frac{hv}{kT}} = 1 + \frac{hv}{kT} \text{ by neglecting higher powers}$$

Then the Planck's law is reduced to

$$E_\lambda = \frac{8\pi kT}{\lambda^4}$$

This is known as Rayleigh Jean's law.

**7. What is Compton effect?**

(AU, Jan 2011)

When a beam of high frequency radiation (X-ray or  $\gamma$ -ray) is scattered by a substance of low atomic number, the scattered radiation consists of two components, one has the same wavelength as the original incident ray and the other has a slightly longer wavelength. The phenomenon of change in the wavelength of scattered X-rays or  $\gamma$ -rays is called Compton shift and the effect is known as Compton effect. It was discovered by A.H.Compton in 1920.

**8. What is Compton wavelength?**

(AU, Jan 2008)

In Compton scattering experiment,

When  $\theta = 90^\circ$ ,  $\cos \theta = 0$ ,

$$\text{Then, } d\lambda = \frac{h}{m_e c} (1 - \cos \theta) = \frac{h}{m_e c} = \frac{6.625 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} = 0.0243 \text{ Å}$$

This is known as Compton wavelength of electron.

9. Give the expression for the change in wavelength of a scattered X-ray photon.

The change in wavelength of a scattered X-ray photon is given by

$$d\lambda = \frac{h}{m_e c} (1 - \cos \theta)$$

Where  $h$  is Planck's constant  $m_e$  the rest mass of electron,  $c$  is the velocity of light and  $\theta$  is the angle of scattered photon.

10. What is wave particle duality?

Experimental results show that light behaves as particle based on photoelectric effect and Compton effect, and as waveform based on interference and diffraction. So, light radiation exhibits both particle and wave nature. Louise de Broglie suggested that an electron or any other particle like proton must also exhibit wave like properties when they are in motion. This property is known as wave-particle duality.

11. What are matter waves?

(AU, Dec 2002)

Louis de Broglie suggested that an electron or any other material particle like proton in motion must also exhibit the wave like properties in addition to particle nature. The waves associated with these material particles in motion are known as matter waves or Louis de Broglie waves.

12. How did de Broglie justify his concept?

(AU, May 2002)

In 1924 Louis de Broglie of France postulated that nature is symmetrical in many ways and the universe is made of radiation (light) and matter (particle).

Experimental results show that light behaves as particle form based on, photoelectric effect and Compton effect, and as waveform based on interference and diffraction.

Louis de Broglie suggested that an electron or any other material particle like proton must also exhibit the wave like properties. The waves associated with these material particles in motion are known as matter waves or Louis de Broglie waves.

13. Write an expression for the wavelength of matter waves? or  
What is de Broglie's wave equation? (AU, May 2006, Jan 2010)

The wavelength of matter wave =  $\frac{h}{mv}$

14. Write an expression for the de Broglie wavelength associated with electrons?

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

$$= \frac{h}{\sqrt{2meV}} = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times V}}$$

$$\lambda = \sqrt{\frac{150}{V}} \text{ Å}$$

Where  $h$  is Planck's constant,  $e$  the charge of electron,  $m$  the mass of electron and  $V$  is the accelerating voltage.

15. State the properties of the matter waves. (AU, Jan 2012)
- i) A material particle will have a matter wave just as a light quantum has a light wave.
  - ii) The wavelength of matter waves is given by  $\lambda = \frac{h}{p} = \frac{h}{mv}$ , where  $m$  is the mass and  $v$  is the velocity of the particle.
  - iii) If  $m$  is large or  $v$  is large, the wavelength associated with the particle is small.
  - iv) The matter waves are thus generated when the particles are in motion.
  - v) The wavelength associated with a particle is independent of any charge associated with it.
  - vi) The confirmation of matter wave assign dual nature to the particle.

**16. What are the applications of de Broglie's idea of matter waves?  
(AU, April 2002)**

- Based on de Broglie's matter waves, we can produce electron wave of very short wavelength. The electron wave is used in electron microscope, which can magnify an object many times compared to optical microscope.
- Schrödinger connected the expressions of de-Broglie wavelength with the classical wave equation for a moving particle and obtained a new wave equation.

**17. What is electron diffraction?**

When a beam of electron of known velocity is passed through a thin gold foil and the resultant beam of electron is made to fall on the photographic plate. When the plate is developed, a symmetrical pattern of concentric rings around a central spot is seen which is similar to X-ray diffraction. Hence this effect is known as electron diffraction.

**18. What is the main application of electron diffraction?**

(AU, Jan 2011)

The main application of electron diffraction is to construct electron microscope, scanning electron microscope, transmission electron microscope and scanning tunneling microscope.

**19. What is Schrödinger wave equation?**

Schrödinger wave equation describes the wave nature of a particle in mathematical form. Schrödinger wave equation is the basic equation for the wave mechanics originally proposed by an Austrian scientist Erwin Schrödinger.

**20. What is a wave function?**

- i) The wave function  $\psi$  is a variable quantity that is associated with a moving particle at any position ( $x, y, z$ ) and at any time  $t$  and it relates the probability of finding the particle at that point and at that time.
- ii) The wave function  $\psi$  can give the probability amplitude of the position of the particle at a time but it cannot predict the exact location of the particle at that time.

**21. Write down Schrödinger time independent and dependent wave equations.** (AU, Jan 2010, 2013, May 2011)

The Schrödinger's time dependent wave equation is

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

Where  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$  is called Laplacian operator

The Schrödinger time independent wave equation is

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

**22. Mention some of the physical significance of the wave function.** (AU, Jan 2003, May 2005)

- i) The variable quantity that characterizes the matter wave is called wave function  $\psi$ .
- ii) The wave function connects the particle and wave nature statistically.
- iii) The wave function  $\psi$  is a variable quantity that is associated with a moving particle at any position  $(x, y, z)$  and at any time  $t$  and it relates the probability of finding the particle at that point and at that time.
- iv) The wave function  $\psi$  can give the probability amplitude of the position of the particle at a time but it cannot predict the exact location of the particle at that time.

**23. What are eigen values and eigen functions?** (AU, Jan 2013)

The wave function  $\psi_n$  and the corresponding energies  $E_n$  are often called as eigen functions and eigen values respectively describing the quantum state of the particle.

The eigen wave function  $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$

The energy eigen values  $E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} = \frac{n^2 h^2}{8ma^2}$

**24. What is Quantum Physics?**

Quantum physics is the study of the behaviour of matter and energy at the molecular, atomic, nuclear, and even smaller microscopic levels. We need quantum mechanics to explain the behaviour of electrons in atoms or solids or the behaviour of atoms in molecules. In the early 20<sup>th</sup> century, it was discovered that the laws that govern macroscopic objects do not function the same in such small realms.

**25. Who developed Quantum Physics?**

The birth of quantum physics is attributed to Max Planck's 1900 paper on blackbody radiation. Development of the field was done by Max Planck, Albert Einstein, Niels Bohr, Werner Heisenberg, Erwin Schrodinger, and many others. Ironically, Albert Einstein had serious theoretical issues with quantum mechanics and tried for many years to disprove or modify it.

**26. How Quantum Physics differs from Classical Physics?**

Classical mechanics is completely definite theory in the sense that the computational procedures do not introduce any statistical uncertainties into the system themselves. Quantum mechanics on the other hand is fundamentally a probabilistic theory.

**27. What is special about Quantum Physics?**

Light waves act like particles and particles act like waves (called wave particle duality). Matter can go from one spot to another without moving through the intervening space (called quantum tunnelling). Information moves instantly across vast distances. In fact, in quantum mechanics we discover that the entire universe is actually a series of probabilities. Fortunately, it breaks down when dealing with large objects, as demonstrated by the Schroedinger's Cat thought experiment.

**REVIEW QUESTIONS****PART - B**

1. What are the basic postulates of quantum theory of radiation? Derive Planck's law of radiation. Hence deduce Wien's law and Rayleigh Jean's law. **(AU, May 2008)**
2. Explain Planck's hypothesis. State and derived Planck's law of radiation. **(AU, Jan 2011, May 2012)**
3. Derive an expression for Planck's radiation law and discuss the same for shorter and longer wavelength. **(AU, Jan 2014)**
4. State Compton effect and derive an expression for the change in wavelength to explain the theory of Compton effect. **(AU, Jan 2011, Dec 2011)**
5. Explain Compton effect and derive an expression for the wavelength of scattered photon. **(AU, May 2007)**
6. What are matter waves? Derive an expression for de Broglie wavelength. What are the characteristics of matter wave? **(AU, Jan 2010, 2012)**
7. Derive time independent and time dependent Schrödinger wave equation. **(AU, Jan 2014)**
8. Derive time dependent Schrödinger wave equation. What are the significances of the wave function? **(AU, Jan 2010, 2012)**
9. Explain the application of Schrödinger wave equation to particle in a box.
10. Using Schrodinger's time independent wave equation normalize the wave functions of electron trapped in a one dimensional box. **(AU, Jan 2014)**
11. Derive time independent Schrödinger equation for a one-dimensional case. Use it to prove that a Particle enclosed in a one-dimensional box has quantized energy values. **(AU, Jan 2004)**
12. What is the principle of Scanning Tunneling Microscope? Explain the construction and working of Scanning Tunneling Microscope with a suitable diagram.

**PROBLEMS**

1. A beam of X-rays are scattered by free electrons. At  $45^\circ$  from the beam direction, the At scattered X-rays have a wavelength of  $0.022\text{\AA}$ . What is the wavelength of the incident beam? (Ans:  $0.0149\text{\AA}$ )
2. X-rays of wavelength  $0.324\text{\AA}$  are scattered by a carbon block. Find the wavelength of scattered X-rays for a scattering angle of  $180^\circ$ . (Ans:  $0.1725\text{\AA}$ ).
3. X-rays of wavelength  $0.3\text{\AA}$  undergoes Compton scattering at an angle of  $60^\circ$ . Find the wavelength of the scattered photon and energy of the recoil electron. (Ans:  $\lambda = 0.3121$ ,  $E = 2.571 \times 10^{-16}\text{J}$ )
4. Calculate the de Broglie wavelength of an electron accelerated to a potential of 2 KV. (Ans:  $0.2744\text{\AA}$ ).
5. An electron is confined to a one-dimensional box of side  $10^{-10}\text{ m}$ . Obtain the first four eigen values of the electron.  
(Ans:  $E_1 = 37.63\text{ eV}$ ,  $E_2 = 150\text{ eV}$ ,  $E_3 = 338\text{ eV}$  and  $E_4 = 602\text{ eV}$ ).