MAA OMWATI DEGREE COLLEGE HASSANPUR (PALWAL)

Notes

B.SC 5th Sem

Quantum Mechanics (Physics)

Chapter

1

ORIGIN OF QUANTUM MECHANICS

1.1. INTRODUCTION

Classical Physics deals primarily with the objects at macroscopic level. Most of the effects with which classical theory is concerned are either directly observable or can be made observable with relatively simple instruments like a microscope, which has resolution of the order of one micron ($\sim 10^{-4}$ m) at the best. Newton's laws of motion form the basis of the most elementary principles of classical mechanics and the equations derived from these laws are suitable for the solution of motion of macroscopic bodies.

During the first few decades of the present century, it became evident (with the discovery of X-rays, radioactivity, photoelectric effect, etc.) that the description of the phenomenon on atomic or sub-atomic scales (microscopic scale) where the lengths are of the order of a few angstroms ($1\ \text{Å} = 10^{-10}$ m) to fermis (1 fermi $= 10^{-15}$ m) do not fit well within the domains of the laws of classical physics. It was recognised that older classical laws do not yield correct results when applied to atoms and electrons (*i.e.* to objects of micro size) without considerable modification of classical motions. In microscopic world, the dynamical variables like energy and momentum did not have the same meaning as that in the case of classical dynamics. Rather these variables were found to have discrete values in different states of an atom and did not change in a continuous manner from one state to the other as one expects under classical laws. These new concepts led to the formulation of a new mechanics called **Quantum Mechanics**, which was found successful in giving satisfactory explanation to many observed facts related to micro objects.

The development of Quantum Mechanics took place in two stages. The first stage began with Max Planck's hypothesis in 1900 that radiation is emitted or absorbed by matter in discrete packets or quanta, each of energy $h\nu$, where ν is the frequency of radiation and h is Planck's constant ($h = 6.6262 \times 10^{-34}$ Js). The theory consisted of a mixture of classical and non-classical (*i.e.* semi-classical) concepts, and was not completely satisfactory.

The second stage began with the development of wave mechanics by Erwin Schrodinger in 1926. This mechanics combines earlier ideas of classical wave theory with Louis de-Broglie's wave particle duality relationship.

1.2.2. Planck's Hypothesis and Planck's Radiation Law

Old Quantum Theory.

For explaining the distribution of energy in the spectrum of a black body, Max Planck, in 1901, put forward quantum theory of heat radiations. According to this theory "A black body radiation chamber can be supposed to be filled up with simple harmonic oscillators (known as Planck's oscillators) and each has a characteristic frequency of oscillations. Planck proposed that energy of such oscillators cannot change continuously but is limited to a discrete set of values such as integral multiples (*i.e.* harmonics) of some small unit of energy E called the quantum of radiation. This quantum of radiation is called a **photon.** Thus according to this hypothesis, each photon has an energy proportional to the frequency ν of oscillator *i.e.*

$$E = h\nu \qquad \text{...(1.3)}$$

where h is the Universal Planck's constant. Its value is equal to

$$6.62 \times 10^{-34} \text{ Joules-sec (Js)}$$

In other words, Planck's quantum hypothesis is consisted of the assumption that the radiation oscillators are not excited to a continuum of energy states, but that these oscillators exchange energy with the surroundings in discrete units, $h\nu$, so that only available energy states of excitation are given by

$$E = n\,h\nu \qquad \text{...(1.4)}$$

where $n = 0, 1, 2, 3, \ldots$ (n is called quantum number)

On the basis of this hypothesis, one can show that the expression for the energy density E_λ in the range $d\lambda$ has the following form

$$E_\lambda \, d\lambda = \frac{8\pi h c}{\lambda^5} \frac{1}{e^{hc/\lambda k_B T} - 1} \, d\lambda \qquad \text{...(1.5)}$$

This is Planck's radiation law in terms of wavelength at a given temperature. This formula fits the experimental curves (Fig. 1.1) very well for the entire wavelength range. Further, the classical expressions, the Wein's law and Rayleigh-Jean's law can also be deduced from it as particular cases.

1.3. PHOTON

In the above section we have seen that Planck hypothesis provided theoretical interpretation of the spectra of black body radiation by assuming that the modes of oscillation in a black body contained only discrete amounts of energy. (This discrete, quantised behaviour of electromagnetic radiations suggests that light waves are transmitted as packets or quanta of energy.)

Einstein succeeded in explaining photoelectric effect by assuming that electromagnetic radiation travels through space in discrete quanta called photons. Thus photon is a quantum of electromagnetic radiations which always travels along straight paths with velocity equal to that of light and zero rest mass.

Properties of Photon

(i) The energy of a photon of frequency ν is $h\nu$.

(ii) A photon behaves like a particle with rest mass equal to zero and mass equal to

$$m = \frac{E}{c^2} = \frac{h\nu}{c^2} = \frac{hc}{\lambda c^2} = \frac{h}{\lambda c}$$

(iii) It possesses not only a definite energy $h\nu$ but also a definite momentum equal to $p = mc = \frac{mc^2}{c} = \frac{E}{c} = h\nu/c$ or h/λ, λ being wavelength associated with radiation and c the velocity of light. h is a universal constant, called Planck's constant.

(iv) Photons are electrically neutral and so are not affected by electric and magnetic field.

1.3.1. Photo-Electric Effect

Photo-electric effect is the phenomenon of emission of electrons from the surface of metals when light of a suitable frequency falls on them. The emitted electrons are called photo-electrons. The basic features of the photo-electric effect are:

(*i*) There is always a characteristic frequency for every metal known as *threshold frequency* (say ν_0) such that the light of frequency less than ν_0 is incapable of emitting electrons from the emitting surface.

(ii) The velocity of the photo-electrons is completely independent of the intensity of incident light but depends on its frequency.

(iii) The rate of emission of photo-electrons is directly proportional to the intensity of the incident light (not on frequency of the incident radiation).

These observations were satisfactorily explained by Einstein in 1905, using Planck's idea of energy quantisation, according to which electromagnetic radiation does not act like a wave but consists of photons of energy $h\nu$. Using this concept Einstein explained the above observations as follows:

When light of certain frequency ν (or quantum of radiation, $h\nu$) falls on metallic surface, a part of its energy is used up to liberate the electrons from the surface (known as work function) and the rest of energy is carried by the emitted electrons as their kinetic energy. This situation can be expressed mathematically as

$$h\nu = \frac{1}{2}mv^2 + \phi_0$$

where ϕ_0 is the work function of the emitting surface and $\frac{1}{2}mv^2$ is the kinetic energy of ejected electrons. The radiation quantum or photon in such collisions interacts with electrons as a light particle. The work function ϕ_0 is related with threshold frequency as

$$\phi_0 = h\nu_0 \quad \text{...(1.6)}$$

where ν_0 is the minimum frequency for which the electron is just emitted from the interior of the metal to the surface without having any kinetic energy. In other words, we can say that with energy $h\nu_0$ the electron is just able to overcome its binding force with the metallic surface, so

$$h\nu = h\nu_0 + mv^2$$

or

$$\frac{1}{2}mv^2 = h(\nu - \nu_0) \quad \text{...(1.7)}$$

This equation is called Einstein's photoelectric equation which clearly explains the experimental observations as follows:

(i) If the frequency of photons ν is less than ν_0 then $\frac{1}{2}mv^2$ *i.e.*, kinetic energy of photo-electrons is negative which is an absurd result, hence the emission of electrons is not possible.

(ii) The kinetic energy $\frac{1}{2}mv^2$ or velocity of photo-electrons depends on the frequency of incident radiation ν and is completely independent of the intensity of radiation. Thus if the frequency of radiation is kept constant and intensity *i.e.*, number of photons incident per unit area of the surface is increased, the number of photo-electrons emitted will increase but there will be no change in velocity of photo-electrons. Hence the photo-electric current is proportional to the intensity of the incident radiation and the increase of intensity does not affect the maximum kinetic energy.

(iii) The number of electrons ejected per unit time depends upon the number of photons falling on the surface per unit area per sec. (*i.e.* intensity). By increasing intensity of light, the number of photons in the incident radiation increases, so the

1.3.2. Compton Effect

A further evidence of the particle nature of electromagnetic radiation was given by A.H. Compton in 1921, while he was investigating the scattering of X-rays by a block of paraffin. He discovered that *when high frequency radiation is scattered by the electrons of the scatterer, then frequency of scattered radiation is smaller than the frequency of the incident wave or the wavelength of scattered radiation is greater than the wavelength of incident radiation*. This phenomenon is called **Compton Effect**. Compton also observed that decrease in frequency of the scattered radiation varies with the angle between the scattered and incident directions.

According to classical theory, the electric field of the incident electromagnetic wave train exerts a force on the atomic electrons in the scattering material and will set them into forced vibrations of the same frequency as that of incident waves. The oscillatory electrons will then emit rays of frequency equal to their own, like an oscillating dipole. Meaning thereby that the scattered rays should have the same wavelength as that of incident waves. This result was not in agreement with the Compton's experiment. *Compton explained the observed phenomenon on the basis of Planck's quantum theory of radiation where radiation consists of quanta or photons with energy $h\nu$.* Compton treated the scattering phenomenon as equivalent to an elastic collision between two particles, the incident light quantum (photon) and an electron of the scatterer. The decrease in frequency of the scattered photon is due to decrease in its energy because a part of the energy of the incident photon is transferred to the electron during collision and hence the scattered photon moves with reduced energy (decrease in energy means decrease in frequency).

Theory of Compton Scattering (Kinematics)

Consider an X-ray photon of frequency ν incident upon a free electron at rest Fig. (1.2). During collision it imparts a part of its energy to the electron setting it into motion. The scattered light quantum (photon) has a smaller energy and hence smaller frequency.

Let the collision be relativistic, *i.e.* mass varies with velocity. The incident photon possesses energy as well as momentum whereas the electron is supposed to be initially at rest and free before collision. As stated above during collision, a part of the energy of incident photon is imparted to the electron which is recoiled with a velocity v and the scattered photon moves with reduced energy and hence lower frequency ν'.

After collision, let the scattered photon and recoil electron make angles ϕ and θ with the direction of incident photon. By applying the usual laws of conservation of energy and linear momentum, the kinematics of the collision process can be worked out as described below:

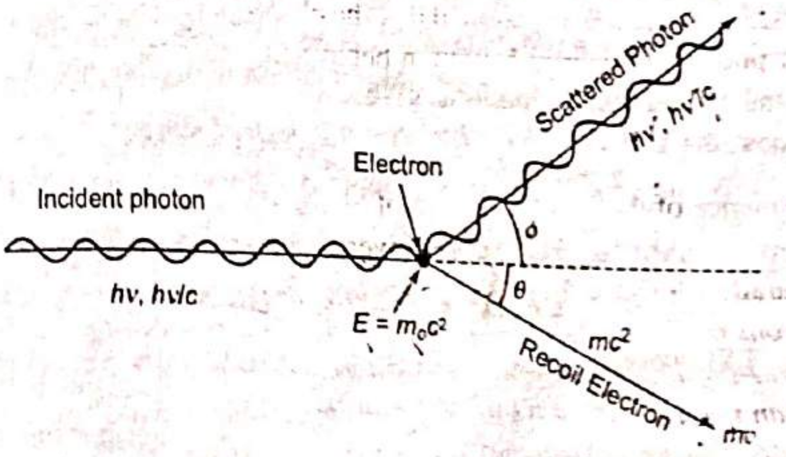

Fig. 1.2.

Before Collision

The energy of incident photon = $h\nu$

The rest energy of the electron = m_0c^2, where m_0 is the rest mass of the electron.

The momentum of the incident photon = $\dfrac{h\nu}{c}$

The momentum of the electron = 0, as it is at rest.

After collision

The energy of the scattered photon = $h\nu'$

The momentum of the scattered photon = $\dfrac{h\nu'}{c}$

The momentum of the recoil electron = mv, where v is the velocity of the electron after collision.

The total energy of the recoil electron (including rest energy) = mc^2, where m is the mass of moving electron given by

$$m = m_0\Big/\sqrt{1-v^2/c^2}$$

From the principle of conservation of energy, we have

Energy of the system (photon + electron) before collision

= Energy of the system after collision

i.e.

$$h\nu + m_0c^2 = h\nu' + mc^2 \qquad ...(1.8)$$

Applying principle of conservation of momentum in the direction of incident photon, we have

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c}\cos\phi + mv\cos\theta \qquad ...(1.9)$$

Applying momentum conservation, perpendicular to the direction of incident photon, we have

$$0 = \frac{h\nu'}{c} \sin \phi - mv \sin \theta \qquad \ldots(1.10)$$

From eqns. (1.9) and (1.10), we can write

$$mv\, c \cos \theta = h\nu - h\nu' \cos \phi$$

$$mv\, c \sin \theta = h\nu' \sin \phi$$

Squaring and adding these equations, give

$$m^2 v^2 c^2 (\cos^2 \theta + \sin^2 \theta) = (h\nu - h\nu' \cos \phi)^2 + (h\nu' \sin \phi)^2$$

or
$$m^2 v^2 c^2 = h^2 (\nu^2 + \nu'^2 \cos^2 \phi - 2\, \nu \nu' \cos \phi) + h^2\, \nu'^2 \sin^2 \phi$$

or
$$m^2 v^2 c^2 = h^2\, [\nu^2 + \nu'^2 (\cos^2 \phi + \sin^2 \phi) - 2\, \nu\, \nu' \cos \phi\,]$$

or
$$m^2 v^2 c^2 = h^2 (\nu^2 + \nu'^2 - 2\, \nu\, \nu' \cos \phi) \qquad \ldots(1.11)$$

From eqn. (1.8), we get

$$mc^2 = h\,(\nu - \nu') + m_0\, c^2$$

Squaring this equation gives

$$m^2 c^4 = h^2 (\nu - \nu')^2 + m_0^2\, c^4 + 2\, m_0\, c^2\, h\, (\nu - \nu')$$

or
$$m^2 c^4 = h^2 (\nu^2 + \nu'^2 - 2\, \nu\, \nu') + 2h\, m_0\, c^2 (\nu - \nu') + m_0^2\, c^4 \qquad \ldots(1.12)$$

Subtracting eqn. (1.11) from eqn. (1.12), we get

$$m^2 c^2 (c^2 - v^2) = 2\, h^2\, \nu\, \nu' (\cos \phi - 1) + 2h\, (\nu - \nu')\, m_0 c^2 + m_0^2\, c^4 \qquad \ldots(1.13)$$

Writing, $m = \dfrac{m_0}{\sqrt{1 - v^2/c^2}}$, eqn. (1.13) becomes

$$m_0^2\, c^4 = 2\, h^2\, \nu\, \nu' (\cos \phi - 1) + 2h\, (\nu - \nu')\, m_0\, c^2 + m_0^2\, c^4$$

or
$$2h\, (\nu - \nu')\, m_0\, c^2 = -\, 2h^2\, \nu\, \nu' (\cos \phi - 1)$$

or
$$\frac{\nu - \nu'}{\nu \nu'} = \frac{h}{m_0 c^2} (1 - \cos \phi)$$

or
$$\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_0 c^2} (1 - \cos \phi) \qquad \ldots(1.14)$$

This expression gives the change in frequency of scattered photon. R.H.S. of eqn. (1.14) is positive giving L.H.S. as positive and hence it follows from eqn. (1.14) that $\nu > \nu'$ *i.e.*, the frequency of incident radiation is greater than the frequency of scattered radiation.

In terms of wavelength $\left(\lambda = \dfrac{c}{\nu}\right)$, the expression (1.14) becomes

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

or
$$\lambda' - \lambda = \Delta\lambda = \frac{h}{m_0 c} (1 - \cos \phi) \qquad \ldots(1.15)$$

(2) When $\phi = \frac{\pi}{2}$, $\cot \frac{\phi}{2} = 1$

Therefore, from eqn. (1.17), $\tan\theta = \frac{1}{1+\alpha}$

$\tan\theta$ being positive, θ lies between 0° and 90°

Also $\Delta\lambda = \frac{h}{m_0 c} = 0.0242$ Å

This means that the photon gets scattered and moves at right angles to the direction of incidence. The change in wavelength is 0.0242 Å while the electron moves in a direction making an angle θ less than $\frac{\pi}{2}$ with the direction of incidence.

(3) When $\phi = \pi$, $\cot\frac{\phi}{2} = 0$, giving

$\tan\theta = 0$ or $\theta = 0$

Also $\Delta\lambda = \frac{2h}{m_0 c} = 0.0484$ Å. This means that the photon reverses its direction with change in wavelength equal to 0.0484 Å, and the electron moves in the forward direction of incident photon. Thus the maximum change in wavelength takes place when the photon gets scattered in the backward direction of incidence.

Kinetic Energy of Scattered (Recoil) Electron in Terms of Photon Scattering Angle (ϕ)

Kinetic energy imparted to the scattered electron from photon = $E_0 = (m - m_0)\, c^2$. This is equal to the decrease in energy of the incident photon. From eqn. (1.8), we have

$$E_0 = h\nu - h\nu'$$

$$= h\nu - h\nu\left[\frac{1}{1+\frac{h\nu}{m_0c^2}(1-\cos\phi)}\right] \qquad \text{(using eqn. (1.14))}$$

$$= \frac{h\nu\left[1+\frac{h\nu}{m_0c^2}(1-\cos\phi)-1\right]}{1+\frac{h\nu}{m_0c^2}(1-\cos\phi)} = h\nu\left[\frac{2\,\alpha\sin^2\phi/2}{1+2\alpha\sin^2\,\phi/2}\right] \quad ...(1.18)$$

where $$\alpha = \frac{h\nu}{m_0c^2}$$

The above expression (1.18) gives K.E. of electrons in terms of angle of scattering of photon.

The energy of the recoil electron will be

$$E_0 = 0 \text{ for } \phi = 0,$$

$$E_0 = \frac{h\nu\alpha}{1+\alpha} \text{ for } \phi = \pi/2$$

and

$$E_0 = h\nu\frac{2\alpha}{1+2\alpha} \text{ for } \phi = \pi$$

Kinetic Energy of Recoil Electron in Terms of Angle of Scattering of Electron (θ)

From eqn. (1.18), we have

$$E_0 = h\nu\left(\frac{2\,\alpha\sin^2\phi/2}{1+2\alpha\sin^2\phi/2}\right)$$

$$= \frac{h\nu\,2\alpha}{\operatorname{cosec}^2\phi/2+2\alpha} = h\nu\frac{2\alpha}{\cot^2\phi/2+1+2\alpha}$$

$$= h\nu\frac{2\alpha}{(1+\alpha)^2\tan^2\theta+(1+2\alpha)} \qquad \text{(using eqn. (1.17))}$$

$$= \frac{h\nu\,2\alpha\cos^2\theta}{(1+\alpha)^2\sin^2\theta+(1+2\alpha)\cos^2\theta}$$

$$= \frac{h\nu\,2\alpha\cos^2\theta}{(\sin^2\theta+\cos^2\theta)+2\,\alpha(\sin^2\theta+\cos^2\theta)+\alpha^2\sin^2\theta}$$

$$= \frac{h\nu\,2\alpha\cos^2\theta}{1+2\alpha+\alpha^2\,(1-\cos^2\theta)}$$

$$= \frac{h\nu\,2\alpha\cos^2\theta}{(1+\alpha)^2-\alpha^2\cos^2\theta} \qquad \text{...(1.19)}$$

From the above discussion, we find that the energy of the scattered electron ranges from zero to $\frac{h\nu\,2\alpha}{1+2\alpha}$ for the scattering angle ϕ of a photon ranging from zero to π (or equivalently for the scattering angle θ of electron ranging from $\frac{\pi}{2}$ to 0). Thus, the maximum energy that the photon can transfer to the electron is $h\nu\frac{2\alpha}{1+2\alpha}$ which is less than $h\nu$ since α is a positive quantity. Hence *the photon cannot transfer its entire energy to the electron.*

Energy of Scattered Photon

Wavelength of the scattered photon from eqn. (1.15) is

$$\lambda' = \lambda + \frac{h}{m_0c}(1-\cos\phi)$$

Therefore frequency of the scattered photon is

$$\nu' = \frac{c}{\lambda'} = \frac{c}{\lambda+\frac{h}{m_0c}(1-\cos\phi)}$$

or

$$\nu' = \frac{c/\lambda}{1+\dfrac{h}{m_0 c\lambda}(1-\cos\phi)} \qquad \text{...(1.20)}$$

$$= \frac{\nu}{1+\alpha(1-\cos\phi)} \qquad \left(\because \alpha = \frac{h}{m_0 c\lambda}\right)$$

Thus the energy of the scattered photon is

$$h\nu' = \frac{h\nu}{1+\alpha(1-\cos\phi)} = \frac{h\nu}{1+2\alpha\sin^2\phi/2} \qquad \text{...(1.21)}$$

Experimental Verification of Compton Effect

If the Compton theory, as described above by the usual kinematics of collision of photon and electron as a two particle collision, is correct then it must be possible to observe the scattered photon and the recoil electron simultaneously. For this purpose, Bothe and Geiger in 1925 conducted the experiment and verified the prediction. The contents of their experiment are described below:

A beam of X-rays was scattered in a small volume of hydrogen gas at atmospheric pressure. The scattered photons and recoil electrons were detected by photon counter and electron counter respectively, arranged opposite to each other and normal to X-ray beam. One of the counters was arranged to respond electrons while the other was closed with a platinum foil and was sensible to photons, as the foil absorbed electrons and allowed X-rays alone to enter the chamber Fig. (1.4).

When a photon enters the chamber, it interacts with the gas in the chamber, thus producing the secondary electrons. It is to be noted that the photon counter does not respond directly to the photon as such striking it; but only directly to secondary electrons:

Now according to Compton theory, if a scattered photon enters the photon counter, a recoil electron must enter the electron counter simultaneously. It was observed that there were about 10 electrons for each scattered photon that were registered by photon counter. This is due to the fact that every photon does not produce a secondary effect. Both of the counters detected simultaneous ionisation in about 10% of the observed cases which is a sufficient indication of the fact that it could merely not be a chance coincidences. Therefore, observed coincidences should only be taken due to simultaneous emission of scattered photon and a recoil electron thereby supporting Compton effect as a two particle collisions.

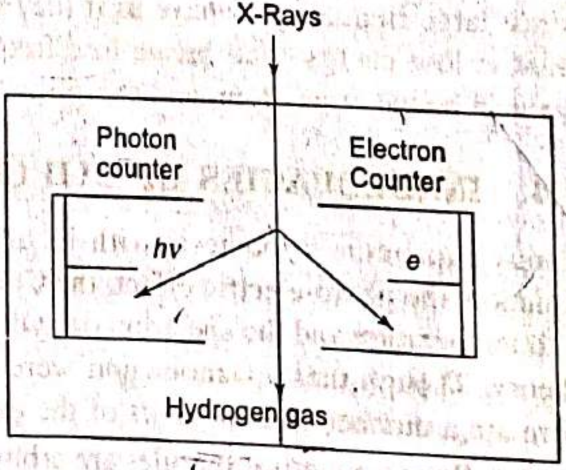

Fig. 1.4.

Further, visible light cannot be used to demonstrate Compton effect. The energy of a visible light photon of wavelength (say)

1.4. INADEQUACIES OF OLD QUANTUM THEORY

Planck's quantum hypothesis with its application to problems of the black body radiation, the photo-electric effect, the Compton effect, the variation of specific heat with temperature and the spectrum of hydrogen atom is now called the Old Quantum Theory. Though these phenomenon were successfully explained by the theory, yet there are a number of drawbacks of the theory, given below:

(*i*) Bohr's quantisation rules are arbitrary. The theory does not provide physical explanation for the assumption.

(*ii*) Bohr's postulate that in stationary orbits, electrons do not radiate energy, was based only on empirical observation and had no theoretical justification.

(*iii*) Old quantum theory could not even explain the spectral lines of simpler systems next to hydrogen atom like hydrogen molecule and normal helium (*iv*) It failed to give any information regarding the transition probabilities and intensity of spectral lines.

(*v*) It could not explain the processes connected with the spin of the electrons and Pauli's exclusion principle.

(*vi*) It could not explain dispersion of light.

(*vii*) The theory cannot be applied to anharmonic systems.

(*viii*) Scattering phenomenon, in general, could not be explained, rather it is out of the purview of old quantum theory.

A breakthrough came from the discovery of the wave nature of matter proposed by de-Broglie in 1925 and the development of Schrodinger's description of these matter waves. The de-Broglie and Schrodinger's methods have been widely used because the basic physical ideas could be explained more easily through the solutions of differential equations involved in mathematical formulations.

Proof of de-Broglie Wave Equation

According to quantum theory, energy of photon (radiation) of frequency ν is

$$E = h\nu$$

If photon is considered to be a particle of mass m, its energy $= mc^2$, then

$$h\nu = mc^2$$

or
$$mc = \frac{h\nu}{c} = \frac{h}{\lambda} \quad \left(\because \lambda = \frac{c}{\nu} \text{ is the wavelength of radiation}\right)$$

$\therefore$
$$\lambda = \frac{h}{mc} = \frac{h}{p} \qquad \text{...(1.23)}$$

where $p = mc$ *is the momentum of the photon.*

de-Broglie assumed that this equation be equally applicable to both the photons of radiation and other material particles.

If m and v be the mass and velocity of the moving particle, then its momentum $p = mv$. Thus the wavelength of the wave associated with material particle is

$$\lambda = \frac{h}{p} = \frac{h}{mv} \qquad \text{...(1.24)}$$

The above equation is known as de-Broglie wave equation and λ is called de-Broglie wavelength. The associated wave is termed as matter or de-Broglie wave.

Eqn. (1.24) can also be derived using the general equation of a standing wave system and the principle of relativity as under.

Consider a material particle *e.g.*, electron or proton as a standing wave system associated with the particle. Let ψ be the quantity that undergoes periodic changes of matter waves at any instant t_0 at the point (x_0, y_0, z_0) then the value of ψ will be represented by

$$\psi = \psi_0 \sin \omega_0 t_0$$

or
$$\psi = \psi_0 \sin 2\pi \nu_0 t_0 \qquad (\omega_0 = 2\pi\nu_0) \qquad \text{...(1.25)}$$

where ψ_0 is the amplitude of the wave at (x_0, y_0, z_0) and ν_0 the frequency of the particle as observed by observer at rest relative to the particle.

Now, if the particle moves with a velocity v along the positive x-direction, then according to inverse Lorentz transformation

$$t_0 = \frac{t + \frac{v}{c^2}x}{\sqrt{1 - \frac{v^2}{c^2}}}$$

and the variation of ψ under this condition is given by

$$\psi = \psi_0 \sin 2\pi \nu_0 \frac{t + \frac{v}{c^2}x}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad \text{...(1.26)}$$

$$\psi = \psi_0 \sin\left\{\frac{2\pi}{\tau}\left(t + \frac{x}{u}\right)\right\} \qquad ...(1.27)$$

where ψ_0 is the amplitude, t the periodic time and u the phase velocity of wave along x-axis.

Comparing eqns (1.26) and (1.27), we get

$$u = \frac{c^2}{v} \qquad ...(1.28)$$

and
$$\frac{1}{\tau} = \nu = \frac{\nu_0}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad ...(1.29)$$

From Einstein's mass energy relation

$$E = m_0 c^2 = h\nu_0$$

or
$$\nu_0 = \frac{m_0 c^2}{h} \qquad ...(1.30)$$

Substituting this in eqn. (1.29), we get

$$\nu = \frac{m_0 c^2}{h} \Big/ \sqrt{1 - \frac{v^2}{c^2}}$$

or
$$\nu = \frac{mc^2}{h} \qquad \left(\because\ m = \frac{m_0}{\sqrt{1 - v^2/c^2}}\right)$$

Thus the wavelength of material particle is given by

$$\lambda = \frac{\text{velocity}}{\text{frequency}} = \frac{u}{\nu} = \frac{\frac{c^2}{v}}{\frac{mc^2}{h}}$$

or
$$\lambda = \frac{h}{mv} \qquad ...(1.31)$$

which is the same as eqn. (1.24). This physically means that a material particle of mass m moving with velocity v has a wave associated with it of wavelength λ given by eqn. (1.31).

Further if E be the kinetic energy of material particle then its momentum $p = \sqrt{2mE}$ (provided $v << c$), then

de-Broglie wavelength is given by

$$\lambda = \frac{h}{\sqrt{2mE}} \qquad ...(1.32)$$

If a charged particle having charge "q" is accelerated through a potential difference V volts, then

$$E = qV$$

and the de-Broglie wavelength for such a particle is given by

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

The method of obtaining an expression for de-Broglie wavelength indicates that a material particle in motion possesses two different velocities, one of which refers to the mechanical motion of the particle represented by v and the other refers to motion of propagation of the phase of the associated wave represented by u. These two velocities are connected by the relation

$$u = \frac{c^2}{v} \qquad ...(1.33)$$

Experimental Verification of Wave-Particle Dualism

The wave nature of material particles was experimentally confirmed independently by Davisson and Germer and by G.P. Thomson.

(a) Davisson and Germer's Experiment

The first experimental evidence for the existence of matter waves was given in 1927 by two American Physicists Davisson and Germer, who succeeded also in measuring the de-Broglie wavelength for slow electrons, accelerated by a low potential difference, by diffraction methods. The experimental set up is shown in Fig. (1.5), where G is the electron gun; T, a single crystal of Nickel chloride, C the collecting chamber.

The electron gun produces the electrons by the process of thermionic emission from a tungsten filament F heated by low tension battery. These electrons are accelerated in an electric field of known potential difference from a high tension battery. The electrons are collimated to a fine beam by suitable slits S_1 and S_2. Thus electron gun is a device by which we get the electrons of known velocity in the form of a fine beam. This beam of electrons is directed in a high vacuum and made to strike a Nickel target T, which is capable of rotation about an axis parallel to the axis of the incident beam.

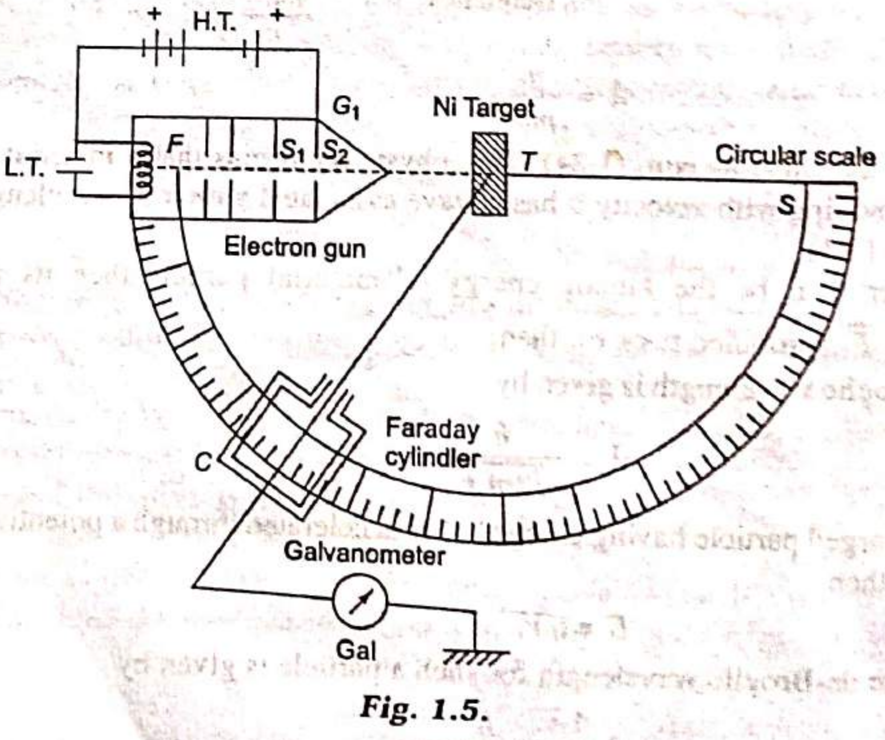

Fig. 1.5.

The electrons are scattered in all directions by the atoms of the Ni crystal. The intensity of the electron beam scattered in a particular direction is measured by allowing it to enter into Faraday cylinder, known as collector C. This is connected to a sensitive galvanometer and is capable of rotation on a graduated circular scale S and is able to receive the reflected electrons in all directions ranging between angles 20° and 90°.

Faraday cylinder is surrounded by a protecting cylinder to which a retarding potential equal to nine-tenths of the accelerating potential is applied so that only the fastest electrons possessing nearly the incident velocity but not the secondary slow electrons produced by collisions with atoms, may enter the cylinder and hence be detected by the galvanometer.

It was observed by Davisson and Germer that there is selective reflection of electron from the Ni crystal, depending on the velocity of the incident electrons. If the velocity of the electrons is gradually increased keeping the source and chamber fixed, it is observed that the distribution of number of electrons reaching the collector follows the curve as shown in Fig. (1.6).

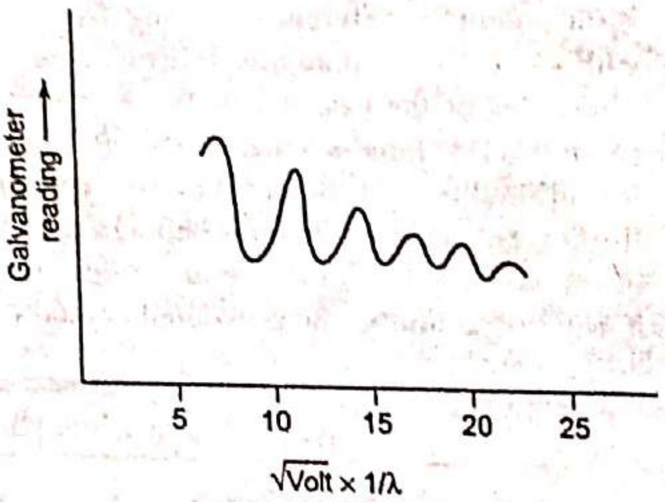

Fig. 1.6.

This selective reflection of the electron beam from the crystal corresponded accurately to diffraction maxima that would be expected in the diffraction of X-rays (whose wavelengths correspond to the equivalent de-Broglie wavelength associated with the moving electron) by the same crystal. If the electrons are assumed simple corpuscles, it is impossible to explain these selective reflections at given velocities. On the other hand, if it is assumed that electrons have waves associated with them, with wave-length varying with velocity in accordance with de-Broglie expression, the selective reflection can be explained using Bragg's law

$$2d \sin \theta = n\lambda \qquad ...(1.34)$$

where n is the order of diffraction pattern and d is the distance between the rows of atoms of the nickel crystal and λ the de-Broglie wavelength of the wave associated with the incident electron beam.

It is therefore possible to calculate the effective wavelength of electrons using Bragg's law. It was observed by Davisson and Germer that when an electron beam accelerated by a potential of 54 V was directed upon a Nickel target,a sharp diffraction maxima appeared in the electron currents. The incident and the scattered beams in this case make an angle of 65° with the family of Bragg's planes. The spacing of planes in this family which can be determined by X-rays diffraction is 0.91 Å. From the above Bragg's eqn. (1.34), taking $n - 1$, we have

$$2 \times 0.91 \text{ Å} \times \sin 65° = 1\lambda$$

(b) G.P. Thomson Experiment

The experimental arrangement of G.P. Thomson is shown in Fig. 1.7 (a). The electrons are produced by passing a current through a filament F and are accelerated by a potential difference ranging from 10,000 to 60,000 volts between anode A cathode C. The apparatus is evacuated to avoid collosion of electrons with the molecules of the gas. A fine beam of electron is obtained by passing the electrons through a fine hole in a metal block B. The electron beam now falls on a thin gold foil 'G' of thickness of the order of 10^{-6} cm. The diffracted beam is allowed to fall on a fluorescent screen S or on a photographic plate P. The photograph of the diffracted beam has a system of concentric rings (See Fig. 1.7 b), similar to that produced by X-ray diffraction in the powdered crystal method.

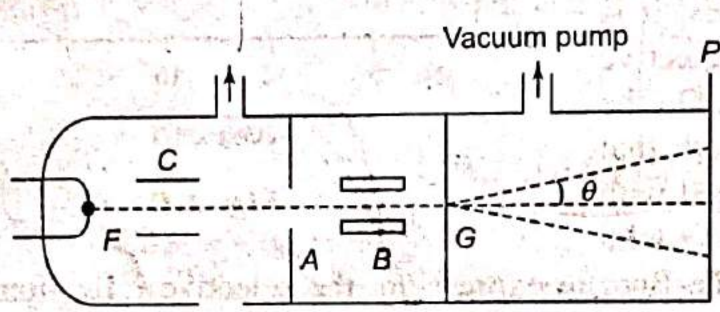

Fig. 1.7. (a)

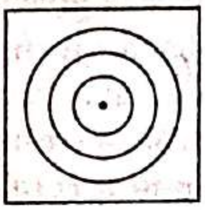

Fig. 1.7. (b)

Calculation of λ from Radii of the Rings

Let $A B$ be the incident beam passing through the gold foil at B. The diffracted beam falls at the point E on the screen at a distance r from the central spot C, as shown in Fig. 1.8. Suppose distance of the film from screen is D and θ is the angle of diffraction.

From Fig. 1.8 we have

$$\tan\theta = \frac{r}{D}$$

Since θ is very small we can write

$$\tan\theta = \theta = \frac{r}{D}$$

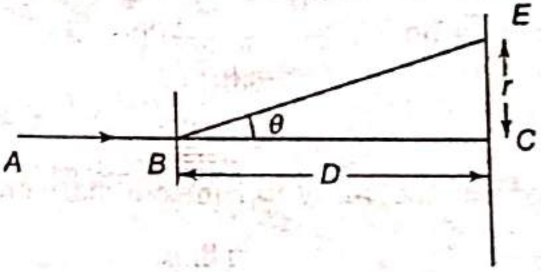

Fig. 1.8.

Thus measuring the radii of the ring and the distance between the film and photographic plate, the angle of diffraction θ can be measured. Further, from Bragg's diffraction relation we have

$$2d\sin\theta = n\lambda$$

where d is the distance between atomic planes and n is the order of spectrum. For small θ we have

$$\sin\theta \equiv \theta = \frac{n\lambda}{2d}$$

Knowing d and the value of θ obtained from above, the wavelength of the diffracted beam can be calculated. The experimental value of λ computed from this pattern was found to be the same as the theoretical value calculated from de-Broglie relation. Thus, the experiment clearly demonstrates the wave nature of electron as diffraction pattern can only be produced by waves.

We further note that in the *same experiment electron showed wave aspect in one part of the experiment and the particle aspects in the other part. In the acceleration process and in the detector it behaves like a particle while in the diffraction process it behaves like a wave*. The dual aspects of material particles are thus required for a complete description of a physical phenomenon. The diffraction experiments with beams of proton, deutrons and other charged particles have also been performed, and all of them establish the validity of the de-Broglie relation.

1.7. GROUP VELOCITY

The velocity with which the centre of mass of wave packet moves is called group velocity or the group velocity may be defined as the velocity with which the centre of mass of slowly varying envelope or packet formed due to a group of waves moves in a medium.

The significance of the group velocity lies in the fact that this is the velocity with which the energy in the wave group is transmitted.

Expression for Group Velocity

Consider a group of waves consisting of only two wave trains of equal amplitudes, but having slightly different frequencies and phase velocities so that they can be represented by the equations

$$\psi_1 = a \cos (\omega_1 t - k_1 x) \quad \text{...(1.42)}$$

and

$$\psi_2 = a \cos (\omega_2 t - k_2 x) \quad \text{...(1.43)}$$

where $\frac{\omega_1}{k_1}$ and $\frac{\omega_2}{k_2}$ represent their respective phase velocities and ψ_1 and ψ_2 are displacement of two waves.

as $$\omega = 2\pi\nu \text{ and } k = \frac{2\pi}{\lambda} \text{ (Propagation constant)}$$

so $$\frac{\omega}{k} = \nu\lambda = \text{Phase velocity or wave velocity}$$

We assume that $\frac{\omega_1}{k} \neq \frac{\omega_2}{k_2}$ *i.e.*, it is a dispersive medium.

The resultant amplitude of the wave may be obtained by adding eqns (1.42) and (1.43) *i.e.*,

$$\psi = \psi_1 + \psi_2 = a\cos(\omega_1 t - k_1 x) + a\cos(\omega_2 t - k_2 x)$$

$$= 2a\cos\left\{\frac{(\omega_1+\omega_2)}{2}t - \frac{(k_1+k_2)}{2}x\right\} \times$$

$$\cos\left\{\left(\frac{\omega_1-\omega_2}{2}\right)t - \left(\frac{k_1-k_2}{2}\right)x\right\} \quad ...(1.44)$$

Let $$\frac{\omega_1+\omega_2}{2} = \omega, \qquad \frac{k_1+k_2}{2} = k.$$

$$\omega_1 - \omega_2 = \Delta\omega;\ k_1 - k_2 = \Delta k$$

Therefore eqn. (1.44) can be written as

$$\psi = 2a\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)\cos(\omega t - kx) \quad ...(1.45)$$

From the above equation of resultant wave it is clear that it consists of two parts:

(*i*) one is a wave of frequency ω, propagation constant k and velocity $v_p = \frac{\omega}{k}$ (phase velocity or wave velocity) and wave length $\frac{2\pi}{k}$.

(*ii*) another is a wave of frequency $\frac{\Delta\omega}{2}$, propagation constant $\frac{\Delta k}{2}$ and velocity $v_g = \frac{\Delta\omega}{\Delta k}$.

Thus ψ consists of wave of the first type and a very slow moving envelope of frequency $\frac{\Delta\omega}{2}$ and propagation constant $\frac{\Delta k}{2}$. While the envelope of the wave packet (dotted line in Fig. 1.11) moves with the group velocity v_g, the individual waves of the packet travels with velocity v_p called phase velocity or wave velocity as explained above is art 1.6. It is the wave group that carries the energy and what we measure experimentally is the group velocity.

$$v_g = \frac{d\omega}{dk}$$

since $\omega = 2\pi\nu$ and $k = 2\pi/\lambda$, so

$$v_g = \frac{2\pi d\nu}{2\pi d\left(\frac{1}{\lambda}\right) d\lambda} = \frac{2\pi d\nu}{-2\pi\left(\frac{1}{\lambda^2}\right)d\lambda} = -\lambda^2\frac{d\nu}{d\lambda}$$

1.9. UNCERTAINTY PRINCIPLE

In classical mechanics a moving particle has a definite momentum and occupies a definite position in space and it is possible to specify precisely both its position and velocity (or momentum) simultaneously. In other words the motion of a classical particle is described by a sharply defined trajectory. During the early century it has become apparent that the classical point of view represents an approximation which is adequate for the objects of appreciable (or macro) size but does not describe satisfactorily the behaviour of the particles of atomic (or micro) dimensions.

The behaviour of particles of atomic dimensions is described on the basis of quantum mechanics, where a particle is represented by a wave packet which moves with group velocity. By the probability interpretation* the particle is likely to be found anywhere within the wave packet. So the position of the particle is uncertain within the size of the wave packet. Again the velocity or momentum of the wave packet is also uncertain as it has velocity spread. This implies that it is impossible to specify accurately both the exact position and velocity or momentum of a particle simultaneously in a wave packet. For small wave packets the position of the particle can be more or less fixed but the velocity or momentum is very uncertain because the velocity spread of small wave packets is very large and conversely for large wave packet (*i.e.* for a wave packet of infinitely large size) the velocity becomes certain but the position is completely uncertain. *So it is impossible to determine the position and momentum of a particle simultaneously accurately.* In other words the trajectory (*i.e.* motion) of a quantum particle is not sharply defined.

Statement

This principle** states that *it is impossible to measure precisely and simultaneously the position of a particle along a particular direction (say x) and its momentum in the same direction, p_x with unlimited accuracy.* If Δx is the uncertainty in the measurement of position and Δp_x is the uncertainty in the measurement of momentum, then according to this principle the product of these two uncertainties is equal to a number of the order $\hbar = \dfrac{h}{2\pi}$ where h being Planck's consiant *i.e.*

$$\Delta x \, \Delta p_x \simeq \hbar \qquad \text{...(1.53)}$$

Similarly $\Delta y \, \Delta p_y \simeq \hbar$ and $\Delta z \Delta p_z \simeq \hbar$ ...(1.54)

Thus if

$$\Delta x = 0, \; \Delta p_x = \frac{\hbar}{0} = \infty$$

and if

$$\Delta p_x = 0, \; \Delta x = \frac{\hbar}{0} = \infty$$

Therefore according to the above relation (1.53), the smaller is the value of Δx *i.e.* the position is more exactly determined, the larger is the value of Δp *i.e.* the momentum is less exactly determined and vice-versa. This relation shows that it is impossible to determine simultaneously both the position and momentum of the particle accurately. The relation is universal and is applicable to all pairs of canonical conjugate physical dynamical variables (in the classical sense) like position and momentum, energy and time, angle and angular momentum etc. whose product has dimensions of action (joule-sec).

Thus if ΔE is the uncertainty in determining the energy of the system and Δt is the uncertainty in determining the time to which this determination refers, then

$$\Delta E \cdot \Delta t \simeq \hbar \qquad \text{...(1.55)}$$

is called the *time energy uncertainty relation i.e.* in any simultaneous determination of the time and energy of a particle, the product of uncertainties is equal to a number of the order of $\hbar$. According to this relation, if the time for which the system remains in a particular energy state is short, then its energy will not be so well defined and for longer stay in a state, the energy will be more well defined. For example, according to Bohr's theory, an electron in an atom goes to an excited state from where it jumps

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* To be discussed later.

** Known as Heisenberg uncertainty principl back to the ground state by emitting a photon of radiation of energy equal to the difference of energy of the two states involved in the transition. If Δt is the time, it remains in this excited state, then Δt will give the error in the measurement of time. Then the error in the measurement of energy cannot be less than $\Delta E = \frac{\hbar}{\Delta t}$. Thus, there will be always an error in the measurement of the energy of the photon. The uncertainty principle in a sense thus sets a limit to the precision with which certain pairs of canonical conjugate physical dynamical variable (in the classical sense), can be defined simultaneously. However, there is no theoretical limit on the accuracy attainable in defining a single variable.

The **exact statement** of uncertainty principle is:

✓ *The product of the uncertainties in determining the position and momentum of a particle simultaneously can never be less than that of the order of* $\hbar/2$.

1.10. EXPERIMENTAL VERIFICATION OF UNCERTAINTY PRINCIPLE (THOUGHT EXPERIMENT)

The validity of uncertainty principle may be illustrated very well by the following hypothetical or thought experiments.

1. Heisenberg's gamma ray microscope: To evaluate the order of limitations in the measurements of the position and momentum of an electron or a photon, Heisenberg proposed an experiment known as Heisenberg's gamma ray microscope.

To measure both the position and the momentum of electron, a high powered γ-ray microscope is set up with a suitable lighting arrangement as shown in Fig. (1.15).

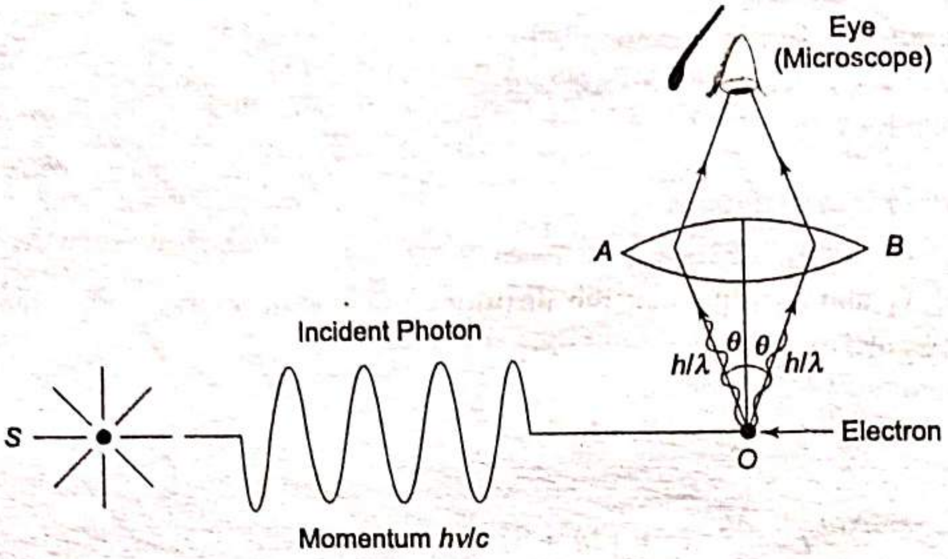

Fig. 1.13.

As the photons from the source S collide with the electrons, some of these bounce (or scattered) into the microscope and enable the observer to see the electron and thus to find out both the position and momentum of the electron at some instant of time. According to classical mechanics, the observer should be able to find out the exact position and momentum of the electrons simultaneously. There are however, two fundamental limitations to such an experiment:

(*i*) **Limitation in determining the position of electron.** According to optical theory, the resolving power of the objective lens of the microscope depends upon the wavelength of light used to illuminate the electron and is given by

$$\Delta x = \frac{\lambda}{2\sin\theta} \tag{1.56}$$

where Δx = minimum distance between two points in the field of view which can be distinguished as separate (*i.e.* minimum distinct measurable distance)

λ = wavelength of scattered photon

θ = semi-vertical angle of the cone (angular aperture is 2θ) of light coming from the illuminated electron.

Thus if the position of the electron changes by less than Δx the microscope will not be able to detect it. To make Δx very small, radiation of very short wavelength such as X-rays or gamma rays should be used. Thus Δx *will be the smallest error or uncertainty in the measurement of the position of the electron.*

(*ii*) **Limitation in measurement of momentum.** In the process of determining the momentum of the electron, the interaction of an electron with γ-ray photon will result in the change of momentum of the electron because of its recoil (Compton effect).

Suppose at any instant, the electron was observed near the point O. It means that at least one photon coming from light source gets scattered by the electron into the microscope causing it to recoil. However, because of finite aperture of the objective lens the electron must be scattered within the angle 2θ so that it could be seen by the microscope. Hence the precise direction in which the electron is scattered into the lens is not known. Now the momentum transferred from the photon to the electron (and hence that of the photon) along the x-axis (*i.e.* perpendicular to the axis of the microscope) can be calculated by Compton effect as under.

Let a photon of momentum $\frac{h\nu}{c}$ strikes an electron initially at rest, so that its initial momentum is zero. The striking photon transfers a momentum mv to the electron and scattes into microscope. Referring to Fig. (1.14), according to principle of conservation of momentum along x-axis, we have

$$\frac{h\nu}{c} = \frac{h\nu'}{c}\cos\alpha + mv\cos\beta$$

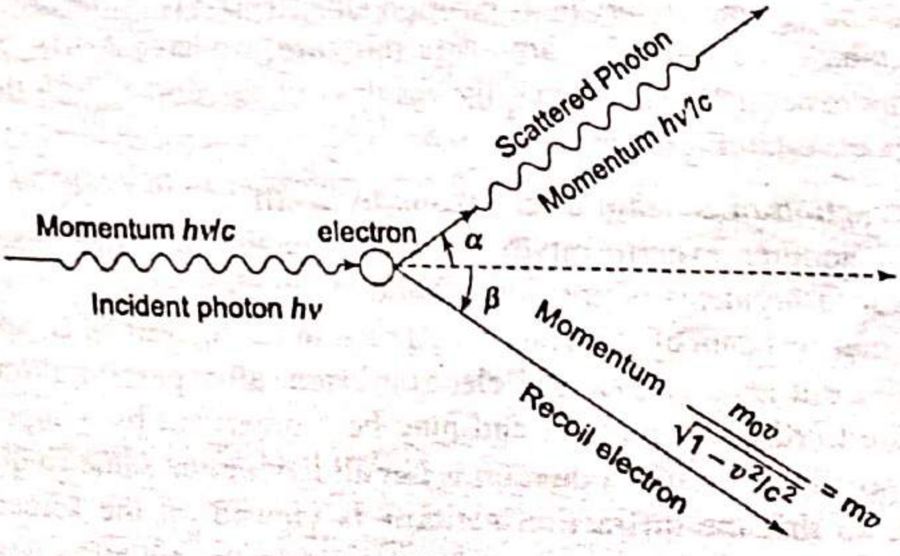

Fig. 1.14.

so the component of momentum along x-axis transferred by the photon to an electron is given by

$$p_x = mv\cos\beta = \frac{h\nu}{c} - \frac{h\nu'}{c}\cos\alpha$$

$$= \frac{h}{c}(\nu - \nu'\cos\alpha)$$

As the limits of angle α inside the microscope are clearly from $(90 - \theta)$ to $(90 + \theta)$, so the spread in the x-component of momentum will be given by

$$\frac{h}{c}[\nu - \nu' \cos(90^\circ - \theta)] \le p_x \le \frac{h}{c}\{\nu - \nu' \cos(90^\circ + \theta)\}$$

or

$$\frac{h}{c}\{\nu - \nu' \sin\theta\} \le p_x \le \frac{h}{c}\{\nu + \nu' \sin\theta\}$$

Thus uncertainty in momentum is given by

$$\Delta p_x = \frac{h}{c}\{\nu + \nu' \sin\theta\} - \frac{h}{c}\{\nu - \nu' \sin\theta\}$$

$$= 2\frac{h}{c}\nu' \sin\theta$$

$$\approx \frac{2h}{\lambda}\sin\theta \tag{1.57}$$

Eqns (1.56) and (1.57) run contrary to each other, because if we try to improve the measurement of the electrons position by decreasing λ and increasing θ, we do it at the cost of the accuracy in the measurement of momentum and vice-versa.

Multiplying eqns. (1.56) and (1.57), we have

$$\Delta x\, \Delta p_x = \frac{\lambda}{2\sin\theta} \cdot \frac{2h\sin\theta}{\lambda}$$

$$\approx h$$

It states that the product of the uncertainty of the x-component of momentum of the electron and the uncertainty in its position along x-axis is of the order of Planck's constant h, which is greater than $\hbar/2$ *i.e.* in this case, we have $\Delta x\, \Delta p_x > \hbar/2$.

Hence this experiment shows that the result is in agreement with the validity of Heisenberg's uncertainty principle.

1.16. EXAMPLE OF TIME-ENERGY UNCERTAINTY

Motion of a one dimensional wave packet provides an example of time-energy uncertainty. Suppose that the wave packet occupies a region of order Δx and let the group velocity be v. The wave packet thus travels with velocity v along the x-axis. However the instant at which it passes a given point of the axis is not determined precisely but has an uncertainty

$$\Delta t \approx \frac{\Delta x}{v} \tag{1.61}$$

Now, if the wave packet is localized to a region Δx, then the spread in the momentum Δp will be given by

$$\Delta p \approx \frac{\hbar}{\Delta x}$$

or

$$\Delta x \approx \frac{\hbar}{\Delta p} \tag{1.62}$$

Putting this in eqn. (1.61), we get

$$\Delta t \approx \frac{\hbar}{\Delta p} \cdot \frac{1}{v}$$

or

$$v \, \Delta t \, \Delta p \approx \hbar$$

But

$$\Delta E = \frac{\partial E}{\partial p} \Delta p \approx v \, \Delta p \qquad \left(E = \frac{p^2}{2m} \right)$$

$\therefore$

$$\Delta E \, \Delta t \approx \hbar$$

This relation indicates that if ΔE is the spread in the energy of a particle then the uncertainty in time at an instant of passage of the particle through a point will be given by

$$\Delta t \approx \frac{h}{\Delta E}$$

Imp.

✓ ***(iii)* The radius of the Bohr's first-orbit (or radius of the hydrogen atom in the ground state).** Suppose Δx and Δp present the uncertainties in the position and momentum of the electron, respectively in the first orbit. According to uncertainty principle, we have

$$\Delta x \, \Delta p \approx \hbar$$

or

$$\Delta p \approx \frac{\hbar}{\Delta x}$$

The uncertainty in the K.E. of the electron may be put as

$$\Delta T = \frac{1}{2} m (\Delta v)^2$$

$$= \frac{1}{2} \frac{(m\Delta v)^2}{m}$$

$$= \frac{1}{2} \frac{(\Delta p)^2}{m}$$

$$\approx \frac{1}{2m} \left(\frac{\hbar}{\Delta x} \right)^2$$

$$\approx \frac{\hbar^2}{2m (\Delta x)^2}$$

The uncertainty in the P.E. of the electron is

$$\Delta V = -\frac{Ze^2}{\Delta x}$$

∴ The uncertainty in the total energy of the electron is

$$\Delta E = \Delta T + \Delta V$$

$$= \frac{\hbar^2}{2m (\Delta x)^2} - \frac{Ze^2}{\Delta x} \qquad (1.63)$$

The uncertainty in the energy will be minimum if

$$\frac{d(\Delta E)}{d(\Delta x)} = 0 \text{ and } \frac{d^2(\Delta E)}{d(\Delta x)^2} = +\text{ve}$$

Eqn. (1.63) yields

$$\frac{d(\Delta E)}{d(\Delta x)} = -\frac{\hbar^2}{m(\Delta x)^3} + \frac{Ze^2}{(\Delta x)^2} \qquad (1.64)$$

For E to be minimum, we must have

$$0 = -\frac{\hbar^2}{m(\Delta x)^3} + \frac{Ze^2}{(\Delta x)^2}$$

or
$$\frac{\hbar^2}{m(\Delta x)^3} = \frac{Ze^2}{(\Delta x)^2}$$

or
$$\Delta x = \frac{\hbar^2}{mZe^2} \tag{1.65}$$

Differentiating eqn. (1.64), we have

$$\frac{d^2(\Delta E)}{d(\Delta x)^2} \approx +\frac{3\hbar^2}{m(\Delta x)^4} - \frac{2Ze^2}{(\Delta x)^3}$$

$$\approx \frac{3\hbar^2}{m(\Delta x)^3\left(\frac{\hbar^2}{mZe^2}\right)} - \frac{2Ze^2}{(\Delta x)^3} \qquad \left(\because \Delta x = \frac{\hbar^2}{mZe^2}\right)$$

$$\approx \frac{3Ze^2}{(\Delta x)^3} - \frac{2Ze^2}{(\Delta x)^3} \approx \frac{Ze^2}{(\Delta x)^3}$$

$$\approx (+)\text{ ve.}$$

As eqn. (1.65) represents the condition that the electron has minimum energy which means that the electron is in the first orbit of hydrogen atom (*i.e.* in the ground state) hence the radius of the first orbit is given by

$$r \approx \Delta x \approx \frac{\hbar^2}{mZe^2} = \frac{h^2}{4\pi^2 mZe^2} \tag{1.66}$$

which is the same as the radius of Bohr's first-orbit.

Chapter

2

SCHRODINGER WAVE EQUATION

2.1. TIME-DEPENDENT SCHRODINGER EQUATION

In this section we would obtain a differential equation, the solution of which describes the behaviour of a particle like electron, proton etc. at certain instant of time t. The solution should describe the wave like behaviour of the particle and also be consistent with uncertainty principle. We assume that the trajectory of a particle should be described by a wave function $\psi(x, t)$ whose magnitude is large in regions where the probability of the occurrence of the particle is large, in other region where the particle is less likely to be found the magnitude of ψ is small. Thus for detailed study of systems we require the equation of motion for $\psi(x, t)$ which was formulated by Erwin Schrodinger in 1926. Schrodinger equation is a fundamental one in quantum mechanism as Newton's equation is in classical mechanics.

One dimensional equation for a free particle

Let us consider a non-relativistic free particle of mass m, velocity v, momentum p_x and energy E is moving along x-axis. By term free particle, it means that no forces are acting on it and its total energy E is entirely kinetic.

$$E = \frac{1}{2}mv^2 = \frac{1}{2m}(mv)^2 = \frac{p_x^2}{2m} \tag{2.1}$$

The moving particle is associated with de-Broglie waves of wavelength λ and frequency ν.

Replacing p_x by $\hbar k$ and E by $\hbar\omega$ in eqn. (2.1), we get

$$\omega = \frac{\hbar k^2}{2m} \tag{2.2}$$

We know that the wave function of a localized free particle is expressed by the wave packet (eqn. (1.39)).Substituting the value of ω from eqn. (2.2), the wave packet for the free-particle can be expressed as

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) \exp\left[i\left(kx - \frac{\hbar k^2}{2m}t\right)\right] dk \tag{2.3}$$

Differentiating $\psi(x, t)$ with respect to t, we get

$$\frac{\partial\psi}{\partial t} = \frac{1}{\sqrt{2\pi}}\left(-\frac{i\hbar}{2m}\right)\int_{-\infty}^{\infty} k^2 A(k) \exp\left[i\left(kx - \frac{\hbar k^2}{2m}t\right)\right] dk$$

2.7 TIME INDEPENDENT OR STATIONARY (STEADY) STATE FORM OF SCHRODINGER WAVE EQUATION

When the Hamiltonian (or potential energy $V(\vec{r}, t)$) does not depend explicitly on time and is a function of $\vec{r}$ only and the total energy E is constant then general solution of Schrodinger eqn. (1.81) for the wave function $\psi(\vec{r}, t)$ can be written as the product of two separate function $u(\vec{r})$, a function only of $\vec{r}$ and $f(t)$, a function only of t, *i.e.*

$$\psi(\vec{r}, t) = u(\vec{r})\, f(t)$$

or briefly

$$\psi = uf$$

From this one gets,

$$\nabla \psi = f \nabla u,$$

$$\nabla^2 \psi = f \nabla^2 u$$

and

$$\frac{\partial \psi}{\partial t} = u \frac{\partial f}{\partial t}$$

Eqn (1.81) now becomes

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

Dividing this equation by the product $u f$, we have

$$\frac{i\hbar}{f} \frac{\partial f}{\partial t} = \frac{1}{u}\left[\frac{-\hbar^2}{2m} \nabla^2 u + V u\right]$$

Since the L.H.S. of this equation is a function of t only while the R.H.S. is a function of $\vec{r}$ only, hence both sides must be equal to the same constant, which we call E. Then the equation for 'f' is

$$\frac{i\hbar}{f} \frac{df}{dt} = E$$

or

$$\frac{df}{f} = \frac{-iE}{\hbar} dt$$

Integrating this gives

$$\log f = -\frac{iE}{\hbar} t + \text{constant}$$

or

$$f(t) = f(0) \exp\left[-\frac{iE}{\hbar} t\right]$$

where $f(0)$ in an arbitrary constant. The equation for u becomes

$$\frac{1}{u}\left[-\frac{\hbar^2}{2m} \nabla^2 u + V u\right] = E$$

or $$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right] u = E\,u \tag{2.19}$$

which is homogeneous equation in u. Now the solution $\psi(\vec{r}, t)$ can be written as

$$\psi(\vec{r}, t) = u\left(\vec{r}\right) e^{-\frac{iEt}{\hbar}} \tag{2.20}$$

1.85

The constant $f(0)$ appearing with $f(t)$ may be chosen to normalise u. For the solution (1.85) one can see that the position probability density

$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2 = |u(\vec{r})|^2$$

is independent of time. Equation (1.84) can be written as

$$Hu(\vec{r}) = Eu(\vec{r})$$

where $u(\vec{r})$ is an eigen function. Normally we represent an eigen function by the symbol $\psi(\vec{r})$, replacing $u(\vec{r})$ by $\psi(\vec{r})$ in the above equation we have.

$$H\psi(\vec{r}) = E\psi(\vec{r}) \tag{2.21}$$

where $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$ is the Hamiltonian operator and E is a number. Equation (2.21) is known as time-independent Schrodinger equation.

2.3. EIGEN VALUES AND EIGEN FUNCTIONS

In the time-independent Schrodinger equation

$$H\psi(r) = E\psi(r)$$

the Hamiltonian operator H operating on the wave function $\psi(r)$ gives a constant E multiplied by the same wave function $\psi(r)$. An equation of the type wherein an operator operating on a function gives a constant and the same function is called *eigen value equation*. In the above equation ψ is said to be an eigenfunction of the operator H that operates on ψ and the constant E multiplying ψ on the right hand side is called the corresponding eigen value of the operator H. A state with a well-defined energy E has a wavefunction of the form (2.20). The solution of time-independent Schrodinger equation can be obtained if the explicit form of the potential $V(r)$ is known. It is found that in general a system has a set of well-defined energy states E_n, for $n = 1, 2, 3, \ldots$ with corresponding wave function $\psi_n(r)$. Including the time dependent part, the wave function of the system is

$$\begin{aligned}\Psi_n(r, t) &= \psi_n(r)\exp\left[-\frac{iE_nt}{\hbar}\right]\\ &= \psi_n(r, 0)\exp\left[-\frac{iE_nt}{\hbar}\right]\end{aligned} \tag{2.22}$$

The probability density $P(r, t)$ is then given by

$$P(r, t) = |\psi_n(r, t)|^2 = |\psi_n(r, 0)|^2 = \text{constant in time}$$

where $n = 1, 2, 3, \ldots$ The states for which probability density is constant in time are called *stationary states.* The time-dependent factor $\exp\left(-\frac{iE_n t}{\hbar}\right)$ of such states are governed by the energy E_n of the particle.

From eqn. (2.22), we have

$$\frac{\partial \psi_n(r,t)}{\partial t} = \psi_n(r,0)\left(-\frac{iE_n}{\hbar}\right)\exp\left(-\frac{iE_n t}{\hbar}\right)$$

or

$$i\hbar\frac{\partial \psi_n(r,t)}{\partial t} = E_n\,\psi_n(r,t) \qquad (2.23)$$

This equation is also an eigenvalue equation with $\psi_n(r, t)$ as the eigenfunction of the operator $i\hbar\frac{\partial}{\partial t}$ with the same eigenvalue E_n, as before. This is to be expected as both operators H and $i\hbar\frac{\partial}{\partial t}$ are energy operators.

Similarly, momentum operator p operating on the plane wave function $\exp[i(kx - \omega t)]$ gives

$$pe^{i(kx-\omega t)} = \left(-i\hbar\frac{\partial}{\partial x}\right)e^{i(kx-\omega t)} = (\hbar k)\,e^{i(kx-\omega t)} \qquad (2.24)$$

This is again an eigenvalue equation with $\exp[i(kx - \omega t)]$ as the eigenfunction of the operator p with the eigenvalue $\hbar k$. Hence $\hbar k$ is called the momentum of the plane wave.

2.4. PHYSICAL SIGNIFICANCE OF WAVE FUNCTION y

The wave function $\psi(\vec{r}, t)$* which is a solution of the Schrodinger equation (2.17) is assumed to provide a quantum mechanical description of the behaviour of a particle

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[*] 1. We have assumed previously that the wave associated with a particle in motion may be represented at any instant t by a complex function $\psi(r, t)$ that is a measure of probability of finding the particle at a given position r. A complex quantity may be expressed as $\psi(\vec{r}, t) = a + ib$ where a and b are real and imaginary parts of ψ and are functions of the variables $(\vec{r}, t)$ and $i = \sqrt{-1}$.

The complex conjugate of ψ *i.e.* ψ^* is given by

$$\psi^*(\vec{r}, t) = a - ib$$

$$\therefore \qquad \psi(\vec{r}, t)\,\psi^*(\vec{r}, t) = a^2 + b^2 \qquad (\because i^2 = -1)$$

The product on the left hand side of the above equation is denoted by

$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2$$

$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2 = a^2 + b^2$$

Contd...

or system of mass m with potential energy V at position $\vec{r}$ and at a given time t. So far the only information available to us regarding the wave function describing the particle (or system) is that the magnitude of ψ is large in the regions where the particle is more likely to be found and small in other regions where the particle is less likely to be found. Therefore ψ may be regarded as a measure of the probability of finding the particle around a particular position. In other words, any meaningful question about the result of an experiment performed upon the system can be answered if the wave function ψ is known. A good agreement with the experimental result and the corresponding calculated result with a given form (or structure) of the wave function is a measure of the correctness (or goodness) of the wave function while the poor agreement between the two results is merely an indication of the fact that the given form (or structure) of the wave function is inappropriate (or not good) and hence has to be suitably modified for its goodness. Hence the success of any model theory (or formulation) is judged by the degree of agreement between the experimental value and the corresponding calculated value based on the form (or structure) of the wave function obtained from the model theory.

The wave function $\psi(r, t)$ however has no physical existence as it can be complex. It cannot be taken as a direct measure of the probability at (r, t) since the probability is real and positive. The statistical interpretation of wave function $\psi(r, t)$ was suggested by Max Born in 1926. He interpreted the product of $\psi(r, t)$ and its complex conjugate ψ^* as the position probability density $P(r, t)$:

$$P(r, t) = \psi^*(r, t)\, \psi(r, t) = |\psi(r, t)|^2 \tag{2.25}$$

Thus if we consider a small element of volume dV defined by the coordinates $(\vec{r}, \vec{r} + d\vec{r})$, then the probability of finding the particle in the volume element dV surrounding the point $\vec{r}$ at time t is given by

$$P(r, t)\, dV = |\psi(r, t)|^2\, dV \tag{2.26}$$

When eqn. (1.92) is integrated over the entire space one should get the total probability, which is unity. Therefore

$$\int_{\infty}^{-\infty} |\psi(r,t)|^2\, dV = 1 \tag{2.27}$$

Contd...

Therefore, we find that the product of ψ and ψ^* is always real and positive if $\psi \neq 0$. Its positive square root is denoted by $|\psi(\vec{r}, t)|$ i.e. modulus of ψ. The position probability density (*i.e.* P) is a real and non-negative quantity and from a complex ψ one can obtain a real and non-negative quantity by multiplying it with its complex conjugate ψ^* and get the product $\psi^* \psi$ as real and non-negative represented as P.

2. The wave function $\psi(\vec{r}, t)$ gives a complete description of the state of the physical system. it is therefore natural to speak of "the state described by the function ψ" or "the state ψ". It may be pointed out that the wave function is arbitrary by a factor whose modulus is equal to unity. In case, this factor is of the form $e^{i\phi}$ whose modulus is equal to unity then ϕ is called the phase of the wave function. Introduction of such a factor with the wave function does not alter the value of any physically observable quantity since the calculation of such a value involves ψ and its complex conjugate ψ^*.

2.5. NORMALISATION OF WAVE FUNCTION

We have seen that the quantity $\psi\psi^* \, dV$ or $|\psi|^2 \, dV$ represents the probability of finding a particle in the given volume element dV.

In physical problems, we come across situations where the particle is bound by forces to a limited region. For example the electron in an atom may be held close to the nucleus by electrostatic forces of attraction, the particle may be confined to a box with non-penetrable walls etc. In such cases the particle is certainly to be found somewhere in the space and hence the probability of finding the particle in the space will be represented by some probability distribution function so that the total probability of finding the particle in the whole of the space considered in a particular problem is *unity*. This may be written mathematically as

$$\int P(\vec{r}, t)\, dV = \int \psi^* (\vec{r}, t)\, \psi(\vec{r}, t)\, dV$$
$$= \int |\psi(r, t)|^2 \, dV = 1 \qquad (2.28)$$

where V is the volume of whole space. In eqn. (2.28) the integration extends over entire (or whole) space in which the particle is confined to move by constraining forces.

A wave function which satisfies eqn. (2.28) is said to be normalized to unity (or briefly normalised). This equation is also referred to as normalisation condition for the wave function $\psi(\vec{r}, t)$.

Generally, ψ is not a normalized wave function but the $\int |\psi(\vec{r}, t)|^2 \, dV$* is finite for $\psi(\vec{r}, t)$ to represent a wave packet (in general for ψ to represent a bound state). ψ is in such a case multiplied by a numerical constant A to give a new function $A\ \psi$ so that $A\ \psi$ (used in place of ψ) satisfies the normalisation condition (2.28). Then it can be seen that the new wave function $A\ \psi$ is also a solution of the wave eqn. (2.21). The numerical constant A is evaluated by using the following condition

$$\int (A\,\psi)^* (A\,\psi)\, dx\, dy\, dz = 1$$

or
$$|A|^2 \int \psi\psi^* \, dx\, dy\, dz = 1 \qquad (2.29)$$

or
$$|A|^2 = \frac{1}{\int \psi\psi^* \, dx\, dy\, dz}$$

where A is termed as normalisation constant. It should be noted that for a plane wave function $e^{i(\vec{k}\cdot\vec{r}-\omega t)}$ the integral (2.28) over infinite volume is not finite. The normalisation of such a wave function requires special consideration.

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* In cartesian coordinates $dV = dx\, dy\, dz$. If ψ is given in polar coordinates, then one should write $dV = r^2\, dr \sin\theta\, d\theta\, d\phi$ where the limits of integration for θ is 0 to π, ϕ is 0 to 2π and the r limit depends on the nature of the physical system (like 0 to ∞, $-\infty$ to 0 or $-\infty$ to ∞).

2.6. ORTHOGONALITY OF WAVE FUNCTIONS CORRESPONDING TO DIFFERENT ENERGY LEVELS

We shall prove the eigenfunctions or wave functions corresponding to different eigenvalues are orthogonal and all eigenvalues are real.

It two wave functions ψ_m and ψ_n belonging to different eigenvalues are such that the integral

$\int \psi_m^* \psi_n \, dV$ or $\int \psi_n^* \psi_m \, dV$ vanishes over entire space for $m \neq n$

Vinash

i.e. $\int \psi_m{}^* \psi_n \, dV = 0$ or $\int \psi_n{}^* \psi_m \, dV = 0$ for $m \neq n$

then the wave functions ψ_m and ψ_n are said to be orthonormal to each other.

Proof: Suppose ψ_m and ψ_n are different solutions of the Schrodinger eqn. (2.21) corresponding to eigenvalues E_m and E_n respectively, then we have

$$\nabla^2 \psi_m + \frac{2m}{\hbar^2} (E_m - V) \psi_m = 0 \tag{2.30}$$

and
$$\nabla^2 \psi_n + \frac{2m}{\hbar^2} (E_n - V) \psi_n = 0 \tag{2.31}$$

The complex conjugate of eqn. (2.30) may be put as follows (assuming V to be real)

$$\nabla^2 \psi_m^* + \frac{2m}{\hbar^2} (E_m{}^* - V) \psi_m{}^* = 0 \tag{2.32}$$

Multiplying eqns (2.31) by $\psi_m{}^*$ and (2.32) by ψ_n, we get

$$\psi_m^* \nabla^2 \psi_n + \frac{2m}{\hbar^2} (E_n - V) \psi_m{}^* \psi_n = 0 \tag{2.33}$$

and
$$\psi_n \nabla^2 \psi_m^* + \frac{2m}{\hbar^2} (E_m{}^* - V) \psi_m{}^* \psi_n = 0 \tag{2.34}$$

Subtracting eqn. (2.34) from eqn. (2.33), we get

$$\psi_m{}^* \nabla^2 \psi_n - \psi_n \nabla^2 \psi_m{}^* + \frac{2m}{\hbar^2} (E_n - E_m{}^*) \psi_m{}^* \psi_n = 0 \tag{2.35}$$

Integrating above equation over the space co-ordinates, we get

$$\iiint (\psi_m{}^* \nabla^2 \psi_n - \psi_n \nabla^2 \psi_m{}^*) \, dV + \frac{2m}{\hbar^2} (E_n - E_m{}^*) \int \psi_m{}^* \psi_n \, dV = 0$$

It is possible to transform the first integral (which is the volume integral) to a surface integral with bounding surface at infinity by using Gauss divergence theorem. This gives

$$\iint_S (\psi_m{}^* \nabla \psi_n - \psi_n{}^* \nabla \psi_m{}^*)_{n_c} \, dS + \frac{2m}{\hbar^2} (E_n - E_m{}^*) \iiint \psi_m{}^* \psi_n \, dV = 0$$

where the subscript n_c denotes the component of the vector within the barcket, in the direction of the outward normal to the element of the area dS.

As ψ_m and ψ_n vanish at the bounding surface at infinity, the first term *i.e.* surface integral becomes equal to zero and we get

$$(E_n - E_m^*) \iiint \psi_m^* \, \psi_n \, dV = 0 \, .$$

For $\quad n \neq m \quad \int \psi_m^* \, \psi_n \, dV = 0 \qquad \text{(as } E_n \neq E_m\text{)}$ (2.36)

Hence the two wave functions ψ_m and ψ_n having this property are said to be orthogonal.

For $n = m$, we have $\int \psi_n^* \, \psi_n \, dV = 1$, if ψ's are normalised to unity which implies $E_n = E_n^*$. *This proves that all the eigenvalues must be real.*

Orthonormal Functions

The set of wave functions which are orthogonal and also normalised are called orthonormal set of wave functions (or complete set of wave functions).

2.7 OPERATOR

An operator is defined as the one when operating on any given function results in a different function. Therefore,

$$g(x) = A\, f(x) \tag{2.37}$$

the operator A operating on $f(x)$ gives the different function $g(x)$. So, in

$$g(x) = A\, f(x) = [f(x)]^2 \tag{2.38}$$

the operator A squares the function $f(x)$. The operator A differentiates the function $f(x)$ with respect to x if

$$g(x) = A\, f(x) = \frac{d}{dx} f(x)$$

Similarly, in

$$g(x) = A\, f(x) = x\, f(x) \qquad (2{:}39)$$

x is an operator. However, a constant is not an operator as it does not change the functional form of the function. An operator is said to be linear if it satisfies the relation

$$A[c_1 f_1(x) + c_2 f_2(x)] = c_1 A\, f_1(x) + c_2 A\, f_2(x) \tag{2.40}$$

where c_1 and c_2 are constants. The sum and difference of operators A and B are defined by

$$(A \pm B) f(x) = A\, f(x) \pm B\, f(x) \tag{2.41}$$

In addition the operators show following properties:

(*i*) Addition is commutative

$$A + B = B + A \tag{2.42}$$

(*ii*) Addition in associative:

$$(A + B) + C = A + (B + C) \tag{2.43}$$

(*iii*) Multiplication is associative:

$$A\,(B + C) f(x) = (A\,B + A\,C) f(x) \tag{2.44}$$

(*iv*) Commutator of operators A and B, denoted by $[A, B]$, is defined as

$$[A, B] = A\,B - B\,A \tag{2.45}$$

It follows that

$$[A, B] = -[B, A] \tag{2.46}$$

The operators A and B are said to commute if $A\,B = B\,A$, *i.e.* $[A\,,\,B] = 0$. Similarly, the operators A and B are said to anticommute if $A\,B + B\,A = 0$. The anticommutator of A with B is usually denoted by $[A\,,\,B]_+$.

As an example of commutator, consider the operators x and (d/dx). The commutator is an operator when operating on function $f\,(x)$ gives

$$\left[x, \frac{d}{dx}\right] f\,(x) = x\frac{df}{dx} - \frac{d}{dx}\,(xf)$$

$$= x\frac{df}{dx} - x\frac{df}{dx} - f\,\frac{d(x)}{dx} = -f$$

Hence

$$\left[x, \frac{d}{dx}\right] = -1 \text{ or } \left[\frac{d}{dx}, x\right] = 1 \tag{2.47}$$

Here the function f has been taken as unity.

Observable

A quantity obtained by the process of observation or measurement on a physical system is known as an observable. The result of the measurement of an observable in a system is expressed by a number. An observable is always a real entity because it is the result of actual measurement.

The act of measurement on a physical system disturbs it. Thus the value of an observable depends on the interaction between the system and the measuring device and is thus spread around some mean value. The value of an observable in general, depends on time. Tims is thus a universal parameter and not itself an observable. If the value of an observable does not change with time, it is a constant of the system. Physical constants such as rest mass and charge of the electron, proton etc belong to this category of observables.

In classical mechanics it is assumed that:

(i) The process of measurement does not disturb the system.
(ii) All the observables of a system are characteristics of the system irrespective of the measuring device.
(iii) Different observable of the system can be measured with maximum accuracy.

In Quantum mechanics.

(i) An observable, although characteristics of the system, depends on the measuring device.
(*ii*) Simultaneous measurement of conjugate variables such as position momentum, time and energy have a fundamental error of measurement given by Heisenberg's uncertainty principle.
(*iii*) Observeable like position co-ordinates, components of linear momentum, the total energy have the same physical meaning as in classical mechanics while observable like spin, symmetry etc. have no equivalent in classical mechanics.

2.10. ONE DIMENSIONAL LINEAR HARMONIC OSCILLATOR

One dimensional oscillator is one of the most important examples of the dynamical system, the applications of which appear in various branches of Physics. For example, it forms the basis of the theory of radiation, the quantization of lattice vibrations etc. and it also illustrates the basic features of a quantum system.

The motion of a point mass attracted to a fixed centre by a force that is proportional to the displacement from the centre, constitute linear harmonic oscillator. A particle undergoing S.H.M. is a typical example of linear harmonic oscillator. Thus for linear harmonic oscillator, the force is represented by

$$F = -kx$$

where k is constant of proportionality (or force (or spring) constant) defined as $\frac{k}{m} = \omega^2$, ω is the angular velocity of oscillator.

The potential energy of harmonic oscillator for the displacement x is

$$V(x) = -\int_0^x F\,dx = -\int_0^x -kx\,dx = \int_0^x kx\,dx = \frac{1}{2}kx^2 + C$$

where C is constant of integration.

At $\qquad x = 0 \quad V(x) = 0$

$\therefore \qquad C = 0$

Therefore $\qquad V(x) = \frac{1}{2}kx^2$

The Schrödinger (time independent) wave equation for an harmonic oscillator is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi = 0 \qquad \text{...(2.62)}$$

Further the frequency ν_0 of a classical oscillator is expressed in terms of its force constant and mass of the particle as

$$\nu_0 = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

or $\qquad k = 4\pi^2\nu_0^2 m$

In dealing with the solution of an equation of the type (2.62), it is convenient to rewrite it in dimensionless form. To do this, a dimensionless variable $y = \alpha x$ and a dimensionless eigenvalue λ are introduced. It is then attempted to put eqn. (2.62) in the form:

$$\frac{d^2\psi}{dy^2} + (\lambda - y^2)\psi = 0 \qquad \text{...(2.63)}$$

The relations for the variable α and eigenvalue λ are obtained by reducing eqn. (2.62) in variable x to the form (2.63) in variable y in the following way:

Now $\qquad y = \alpha x \quad \Rightarrow \quad \frac{dy}{dx} = \alpha$

$$\therefore \qquad \frac{d\psi}{dx} = \frac{d\psi}{dx}\frac{dy}{dx} = \alpha\frac{d\psi}{dy}$$

and $$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \alpha\frac{d}{dx}\left(\frac{d\psi}{dy}\right) = \alpha\frac{d}{dy}\left(\frac{d\psi}{dx}\right) = \alpha^2\frac{d^2\psi}{dy^2}$$

Eqn. (2.62), in terms of variable y, becomes

$$\alpha^2 \frac{d^2\psi}{dy^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}k\frac{y^2}{\alpha^2}\right)\psi = 0$$

or $$\frac{d^2\psi}{dy^2} + \left[\frac{2mE}{\hbar^2}\cdot\frac{1}{\alpha^2} - \frac{km}{\hbar^2}\cdot\frac{1}{\alpha^4}y^2\right]\psi = 0 \qquad \text{...(2.64)}$$

Comparison of eqn. (2.64) with eqn. (2.63) gives

$$\alpha^4 = \frac{km}{\hbar^2} \text{ and } [redacted]$$

$$\lambda = \frac{2mE}{\hbar^2}\cdot\frac{1}{\alpha^2} = \frac{2mE}{\hbar^2}\cdot\frac{\hbar}{\sqrt{km}} = \frac{2E}{\hbar}\left(\frac{m}{k}\right)^{1/2} = \frac{2E}{\hbar\omega} \qquad \text{...(2.65)}$$

Eigenvalues of Harmonic Oscillator

As we have seen above that in order to have a satisfactory wave function, the power series (2.74) must terminate at some value of r. This can be achieved if the coefficient a_r is zero, so that the subsequent coefficients a_{r+2}, a_{r+4} ... etc. are identically equal to zero. Thus the numerator in the recursion formula (2.78) would be equal to zero *i.e.*

$$2s + 2r + 1 - \lambda = 0$$

i.e.
$$\lambda = 2s + 2r + 1 \qquad \text{...(2.80)}$$

For $s = 0$, we have

$$\lambda = 2r + 1$$

For $s = 1$, we have

$$\lambda = 2r + 3$$

Thus eqn. (2.80) may be written in a more general way to cover both cases ($s = 0$, $s = 1$) in terms of a quantum number n.

$$\lambda = 2n + 1 \text{ where } n = 0, 1, 2 \qquad \text{...(2.81)}$$

or
$$(2n + 1) = \frac{2E_n}{\hbar\omega} \qquad \text{(using eqn. (2.65) for } \lambda)$$

or
$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad \text{...(2.82)}$$

Quantisation of Energy

Thus the allowed integral values of n lead to certain discrete values of energy (*i.e. quantised*) given by eqn. (2.82) known as eigenvalues of harmonic oscillator. These eigenvalues (energy levels) are $\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega$... which are equally separated by

$\hbar\omega$ (characteristics of harmonic oscillations) and quantised. These energy levels are shown in Fig. 2.1. The parabola is due to potential energy of the particle.

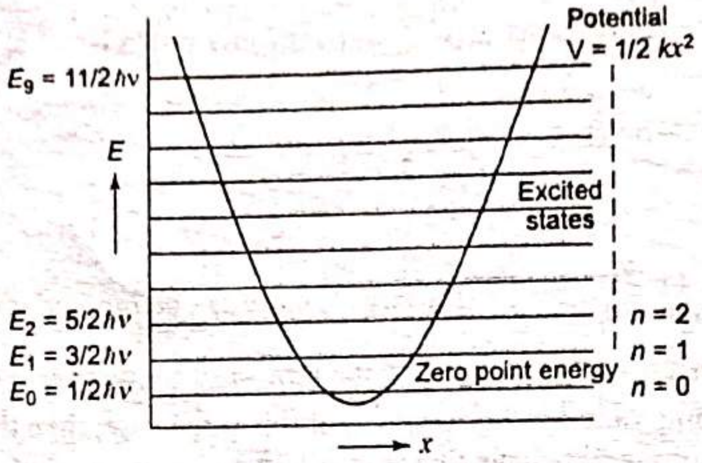

Fig. 2.1. *Energy levels of Harmonic Oscillator.*

Zero Point Energy and its Significance

For ground state which is the lowest energy state for $n = 0$, the energy eigenvalue E_0 is (putting $n = 0$ in eqn. 2.82),

$$E_0 = \frac{1}{2}\hbar\omega \qquad \text{...(2.83)}$$

This is called *zero point energy*. This result is different from old quantum theory according to which $E_n = n\hbar\omega$ *i.e.* the energy levels are equally separated by $\hbar\omega$, in agreement with the energy separation in the present case but the oscillator has zero energy for ground state ($n = 0$).

A comparison of this result, with the result $E_n = n\hbar\omega$ obtained by old quantum theory, shows that the only difference is that all the equally spaced energy levels are shifted upward by an amount equal to half the separation of energy levels *i.e.* $\frac{1}{2}\hbar\omega$. Thus it is clear that even in the lowest state, the harmonic oscillator has energy greater than that it would have if it were at rest in the equilibrium position. Associated with the minimum energy state is the 'zero point motion' of the particle *i.e.* the particle does not cease motion about the origin but remains spread out. Furthermore the existence of zero point energy is in agreement with experiment and is characteristics of quantum mechanics and is related to uncertainty principle.

It follows from eqns. (2.82) and (2.78) that n is the highest value of $s + r$ in the series (2.74) for H (y). If we denote the polynomial corresponding to n by $H_n(y)$, we see that H_n is of order n in y and is a completely even or odd polynomial according to n is even or odd.

Hermite Polynomials

The nth Hermite polynomial $H_n(y)$ for a given n, is a solution of the differential eqn. (2.73) which can be rewritten in terms of n, using eqn. (2.80), in the form

$$H_n'' + 2y\,H_n' + 2n\,H_n = 0 \quad \text{(primes over } H \text{ refer to differentiation)} \quad \text{...(2.84)}$$

We have already discussed the series method for solving eqn. (2.73) to get H_n. The detailed properties of H_n can be studied using recursion relations which can be derived by series method (details not discussed here). We shall rather discuss here a more

Chapter

3

APPLICATIONS OF SCHRODINGER WAVE EQUATION TO ONE DIMENSIONAL PROBLEMS

3.1 FREE PARTICLE IN ONE DIMENSIONAL BOX (ONE DIMENSIONAL RECTANGULAR POTENTIAL WELL WITH REFLECTING WALLS OR OF INFINITE POTENTIAL HEIGHT)

In quantum mechanics, a box means a system in which a particle is free so that the potential energy V of the particle is zero within a closed region (i.e. the size of the box) and infinite everywhere. One dimensional box means the particle moves only along a straight line say along x-axis. Also

(i) The walls of the box are non-penetrable *so that there is no chance of finding the particle outside the box.*

(ii) The walls of the box are rigid and perfectly elastic, *so that total energy E of the particle remains constant as the particle rebounds with the same kinetic energy after making the elastic collision with the wall.*

For one dimensional box of length a, mathematically we can write for the potential energy $V(x)$ as

$$V(x)=\begin{cases} 0 \text{ for } 0 < x < a \text{ (inside the box)} \\ \infty \text{ for } x < 0 \text{ and } x > a \text{ (outside the box)} \end{cases} \tag{3.1}$$

Schrödinger Wave Equation

The Schrödinger equation for the wave function of a particle of mass m constrained to move along a straight line (x-axis) is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{3.2}$$

If the total energy of the particle has fixed value E, (as in the present case), the time dependence of ψ is given by

$$\psi(x,t) = \psi(x,0)\, e^{\frac{-iEt}{\hbar}} = \psi(x)\, e^{\frac{iEt}{\hbar}} \tag{3.3}$$

and $\psi(x)$ satisfies the time independent Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(\mathrm{E} - V(x)\right)\psi = 0 \tag{3.4}$$

Now we shall find the solution of this eqn. (3.4) for the given potential function $V(x)$ of the form given by eqn. (3.1), shown in Fig. 3.1.

Zero and Negative Values of n not Permissible

It may be emphasised here that the constant A cannot be taken as zero because in that case B = – A will also become zero and hence the solution (3.8) will make the wave function vanish everywhere which is physically uninteresting. Further n is not taken to be equal to zero or negative because $n = 0$, makes $k = 0$, which means that the momentum and hence the kinetic energy of the particle is zero *i.e.* the particle is at rest for all times which is not physically true. Also $k = 0$ (like $A = -B = 0$) gives $\psi(x) = 0$ which means that probability density $|\psi|^2 = 0$ *i.e.* the particle is not in the box.

The negative values of n simply repeat the corresponding values for positive n and do not give independent solutions.

Thus the solution of eqn. (3.7) can be written as

$$\psi(x) = A\,(e^{ikx} - e^{-ikx}) = 2iA \sin kx$$

or

$$\psi(x) = C \sin kx \tag{3.12}$$

where C = 2*i*A is another constant.

Evaluation of C

To evaluate the constant C, we apply the normalisation condition *i.e.* the total probability of finding the particle inside the box is unity.

$$\therefore \qquad \int_0^a |\psi(x)|^2\, dx = 1$$

Using eqn. (3.12), we get

$$|C|^2 \int_0^a \sin^2 kx\, dx = 1$$

or

$$|C|^2 \int_0^a \sin^2 \frac{n\pi}{a} x\, dx = 1 \qquad \text{(by eqn. (3.11))}$$

or

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

or

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

or $$|C|^2 \frac{1}{2} x \Big|_0^a - \frac{1}{2}|C|^2 \cdot \frac{a}{2n\pi} \cdot \sin \frac{2n\pi x}{a} \Big|_0^a = 1$$

or $$|C|^2 \frac{a}{2} - 0 = 1$$

or $$C = \sqrt{\frac{2}{a}}$$

Hence the normalised wave function is

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x \tag{3.13}$$

Eigen Functions

Using the above equation, we can write the various *eigenfunctions* as

$$y_1 = \left(\frac{2}{a}\right)^{1/2} \sin \frac{\pi}{a} x$$

$$y_2 = \left(\frac{2}{a}\right)^{1/2} \sin \frac{2\pi}{a} x$$

……………………………………

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$$y_n = \left(\frac{2}{a}\right)^{1/2} \sin \frac{n\pi}{a} x$$

These eigen functions are plotted in Fig. (3.2)

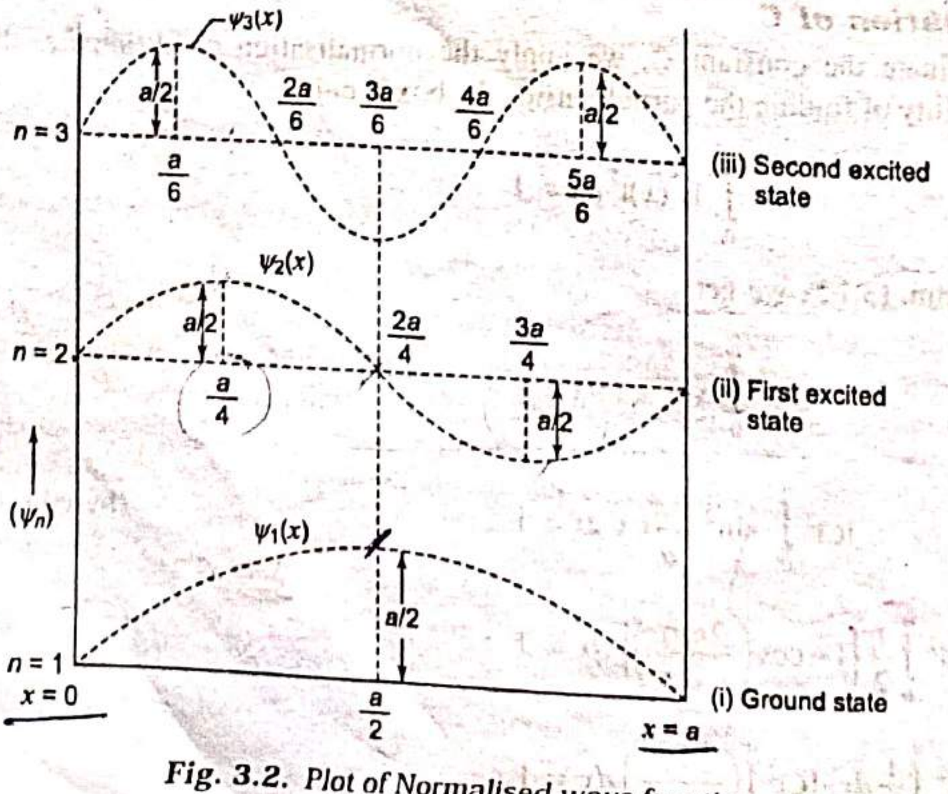

Fig. 3.2. Plot of Normalised wave function.

Energy Eigenvalues

For finding energy eigenvalues, we have from eqn. (3.11)

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

Putting the value of k^2 in eqn. (3.6), we have

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

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad (3.14)$$

Also momentum of the particle inside the box, $p_n = \hbar k$

$$= \hbar\frac{n\pi}{a} = \frac{nh}{2a} \qquad (3.15)$$

where $n = 1, 2, 3...$ and $\hbar = h/2\pi$

Thus we find that energy and momentum of the particle in a box consists of a set of discrete values corresponding to different values of n where the number n is called quantum number. Thus momentum and energy of a particle in a box are quantised. The discrete set of E values are called energy levels. The assembly of energy eigenvalues (in increasing order) of a particle is called *energy spectrum* (or energy levels). Thus the energy spectrum of particle in box is discrete. If a particle is described by a wave function with a certain n value, it is said to be in the quantum state n. The quantum state with lowest n (= 1) is called ground state while states with higher n (= 2, 3, ...) are called excited states (Fig. 3.3). In general, the imposition of the boundary conditions make the energy eigenvalue spectrum discrete. It should be noted that for a free particle without boundaries the spectrum is continuous. One can observe from eqn. (3.14) that for particle in a box if $a \to \infty$, then the spacing between the energy levels approaches to zero and hence the spectrum approaches to a continuous set of energy values implying that the particle behaves as if it is free *i.e.* without any box (or boundary conditions).

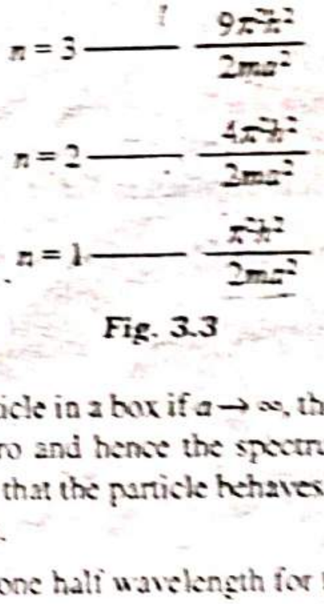

Fig. 3.3

Discussion: From Fig. (3.2) it is clear that there is only one half wavelength for the lowest energy state called zero point energy while the successive energy states differ by an additional half wavelength. There are certain points between $0 \le x \le a$ at which the wave function vanishes or attains maximum value. The points where $\psi(x) = 0$ are called *nodes* and the points where $\psi(x)$ = maximum are called antinodes. Thus

For nodes: $\psi(x) = 0$ For the nth quantum state, the nodes occur for

$$\sin\frac{n\pi x}{a} = 0$$

or
$$\frac{n\pi x}{a} = p\pi, \; p = 0, 1, 2, \ldots n$$

$\therefore$
$$x = \frac{pa}{n} \tag{3.16}$$

or nodes occur at $x = 0, \frac{a}{n}, \frac{2a}{n}, \ldots \frac{na}{n}$

For Antinodes $\psi(x) = maximum$

Maximum value of $\sin \frac{n\pi x}{a} = 1$.

i.e. for an anti-node $\psi_n(x) = \left(\frac{2}{a}\right)^{1/2} \times 1$

$\therefore$ For the nth quantum state the antinodes occur for

$$\sin \frac{n\pi x}{a} = 1 = \sin (2p + 1) \frac{\pi}{2}$$

$\therefore$
$$x = \frac{(2p+1)a}{2n}; \quad p = 0, 1, 2, \ldots \tag{3.17}$$

$\therefore$ antinodes occur at

$$x = \frac{a}{2n}, \frac{3a}{2n}, \frac{5a}{2n}, \ldots \frac{(2n-1)a}{2n}$$

When $n = 1$ node occurs at $x = 0$ and $x = a$

and antinodes occur at $x = a/2$

This is depicted in Fig. 3.2 (*i*)

When $n = 2$ nodes occur at $x = 0, x = \frac{a}{2}, x = a$

antinodes occur at $x = \frac{a}{4}, x = \frac{3a}{4}$

This is depicted in Fig. 3.2 (*ii*)

When $n = 3$ nodes occur at $x = 0, x = \frac{a}{3}, x = \frac{2a}{3}; x = a$

antinodes occur at $x = \frac{a}{6}, x = \frac{3a}{6}, x = \frac{5a}{6}$

This is shown in Fig. 3.2 (*iii*).

In terms of probability density, an antinode is a point of maximum probability density and a node is a point of zero probability density. Therefore, for the nth quantum state, we find that there are n antinodes, *i.e.* there are n equally probable positions in the box at which the particle is most likely to be found. Similarly, there are $(n-1)$ nodes, each node lying in between two antinodes *i.e.* there are $(n-1)$ equally spaced positions where the probability of finding the particle is zero. Of course, the two positions $x = 0$ and $x = a$ are permanent positions of nodes.

In the ground state $n = 1$, the position of maximum probability is given by $x = \frac{a}{2}$. For the first excited state $n = 2$, the probability is maximum for $x = \frac{a}{4}$ and $x = \frac{3a}{4}$ but the probability for $x = \frac{a}{2}$ is zero.

The probability of locating the particle at $x = 0$ or $x = a$ *i.e.* at the walls is always zero (outside the walls it is already zero).

Zero Point Energy for a Particle in One Dimensional Box

For a free particle in an one dimensional box of length a, the nth wave function and energy eigenvalues are given by

$$\psi_n(x) = \left(\frac{2}{a}\right)^{1/2} \sin \frac{n\pi}{a} x$$

and $$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \text{ respectively.}$$

Now for $n = 0$, $E_0 = 0$ and $\psi_0(x) = 0$.

It means that for $E_0 = 0$, the probability of the particle being within the box is nil *i.e.* there can be no particle in the box. Hence, if the particle is in the box, n cannot be zero, So the smallest possible value of n is $n = 1$ for which

$$\psi_1(x) = \left(\frac{2}{a}\right)^{1/2} \sin \frac{\pi x}{a}$$

and $$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

Thus the minimum energy that the particle can have is $\frac{\pi^2\hbar^2}{2ma^2}$. In other words, even when the temperature of the box is reduced to 0 K, the total energy will still be E_1 and will not be zero. Therefore $E = \frac{\pi^2\hbar^2}{2ma^2}$ is called zero point energy of the particle.

If m is very large *i.e.* for a heavy particle or if a is very large *i.e.* for a box of the very large size, the zero point energy is almost zero.

2.2. POTENTIAL STEP OR SINGLE STEP BARRIER ($E > V_0$)

When a force field (or potential) acting on a particle is zero everywhere except in a limited region, it is known as potential step or a single step barrier. In the case of potential step, the potential function undergoes only one discontinuous change at $x = 0$ as shown in Fig. (3.4) and hence the potential function of a potential step can be represented as

$$V(x) = \begin{cases} 0 \text{ for } x < 0 \\ V_0 \text{ for } x \geq 0 \end{cases}$$

$E > V_0$

One Dimensional Potential Barrier $E > V_0$

Now let us consider that a particle having energy E is incident on the barrier from left (Region I) on the potential step $V(x) = V_0$ at $x = 0$, the origin of the x-axis.

The potential energy of the particle is zero when it is to the left of the step *i.e.* left of the origin O and the potential energy $V(x) = V_0$ to the right of the step or the origin

$$\therefore \quad V(x) = 0 \text{ for } x < 0 \qquad \text{Region I}$$
$$= V_0 \text{ for } x > 0 \qquad \text{Region II}$$

Now as that the total energy of the incident particle is greater than V_0, the value of step potential *i.e.* $E > V_0$, so $\sqrt{2m(E - V_o)}$ will be positive and real and classically the particle can penetrate the barrier and move (with reduced kinetic energy) in the positive x-direction *i.e.* in this case the particle can be in region $x > 0$ as well as $x < 0$.

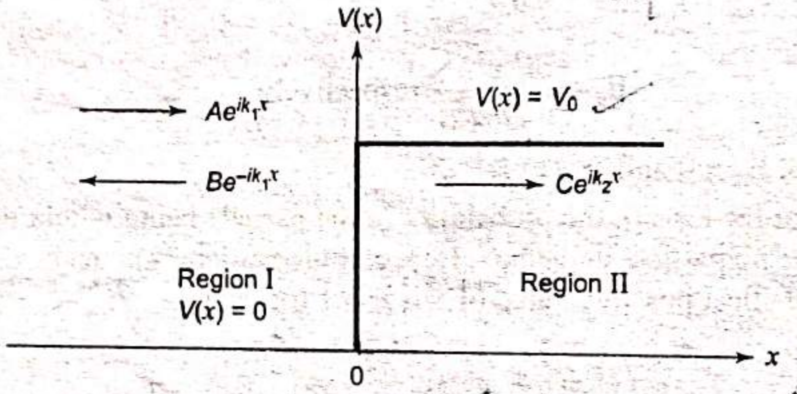

Fig. 3.4. *Potential step.*

Quantum mechanically, the particles behave like a wave moving from left to right and face a sudden change in potential at a point of discontinuity at $x = 0$, we will show that for $E > V_0$, the particle may undergo partial reflection and partial transmission at $x = 0$ and for $E < V_0$ although reflection coefficient is unity, the wave function is non-zero in the region $x > 0$, implying that there is a finite probability of finding the particle in the region $x > 0$. The problem is analogous to light wave striking a sheet of glass, thereby the incident wave is partly transmitted.

The one dimensional time independent Schrödinger equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0 \tag{3.18}$$

Now to solve the problem let us write the Schrödinger equation for the two regions. (Fig. 3.4)

Case I. $E > V_0$, the Schrödinger equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \text{ for } x < 0 \tag{3.19}$$

and
$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\,\psi = 0 \text{ for } x > 0 \tag{3.20}$$

Putting
$$\sqrt{\frac{2mE}{\hbar^2}} = k_1$$

and $\sqrt{\frac{2m(E-V_0)}{\hbar^2}} = k_2$ in the above equations,

We have

$$\frac{d^2\psi}{dx^2} + k_1^2\psi = 0 \qquad \text{for } x < 0 \tag{3.21}$$

$$\frac{d^2\psi}{dx^2} + k_2^2\psi = 0 \qquad \text{for } x > 0 \tag{3.22}$$

General solutions of eqns. (3.21) and (3.22) may be written as

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \qquad \text{for } x < 0 \tag{3.23}$$

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x} \qquad \text{for } x > 0 \tag{3.24}$$

where ψ_1 and ψ_2 are the wave functions in regions I and II respectively; A, B, C and D are constants and can be determined by using the usual boundary conditions on ψ and $\frac{d\psi}{dx}$ at the point of discontinuity in the potential at $x = 0$.

In these two equations, the wave function is made up of two terms, the first term of eqn. (3.23) is a wave travelling along + ve x-axis (*incident wave*), second term is a wave moving along – ve x-axis (*reflected wave at the interface*) in the region I. In eqn. (3.24), the first term is again a wave advancing in the positive direction of x-axis in the region II (*transmitted wave*) whereas the second term represents a wave moving in the negative direction of x-axis in the region II (*reflected wave*). As there occurs discontinuity in the potential only at $x = 0$ in the region II and thereafter there occurs no discontinuity, it means that the reflection will not take place in region II and hence $D = 0$. Consequently, the second term of eqn. (3.24) in discarded in region II. Hence the eqn. (3.24) becomes as

$$\psi_2 = Ce^{ik_2x} \text{ for } x > 0 \tag{3.25}$$

Alternatively A, B, C represent the amplitudes of incident, reflected and transmitted waves respectively.

Determination of Constants

These amplitudes (A, B and C) can be determined by using the boundary conditions, which require that the wave function and its derivative must be continuous at the boundary *i.e.* at $x = 0$ *i.e.*

$$\psi_1 = \psi_2 \qquad (\text{at } x = 0)$$

and

$$\frac{\partial\psi_1}{\partial x} = \frac{\partial\psi_2}{\partial x} \qquad (\text{at } x = 0)$$

Putting $x = 0$ in eqns. (3.23) and (3.25) and equating $\psi_1 = \psi_2$, we get

$$A + B = C \tag{3.26}$$

Now differentiating eqns (3.23) and (3.24), we have

$$\frac{\partial\psi_1}{\partial x} = ik_1[Ae^{ik_1x} - Be^{-ik_1x}] \tag{3.27}$$

and $$\frac{\partial \psi_2}{\partial x} = ik_2 Ce^{ik_2 x} \qquad (3.28)$$

Putting $x = 0$ in eqns (3.27) and (3.28) and equating $\frac{\partial \psi_1}{\partial x} = \frac{\partial \psi_2}{\partial x}$, we have

$$ik_1 (A - B) = ik_2 C \qquad (3.29)$$

Since there are only two eqns (3.26) and (3.27) connecting constants A, B and C and hence they cannot be uniquely determined. We will, therefore, determine B and C in terms of A.

Substituting for C from eqn. (3.26) in eqn. (3.29), we get

$$k_1(A - B) = k_2(A + B)$$

or $$(k_1 - k_2)A = (k_1 + k_2)B$$

or $$B = \frac{(k_1 - k_2)A}{(k_1 + k_2)} \qquad (3.30)$$

Putting this value of B in eqn. (3.26), we have

$$C = A + \frac{(k_1 + k_2)A}{(k_1 + k_2)}$$

$$= \frac{(k_1 + k_2 + k_1 - k_2)A}{k_1 + k_2} = \frac{2k_1}{k_1 + k_2} A \qquad (3.31)$$

i.e. the amplitudes of reflected and transmitted waves are described in terms of the amplitude of incident wave. The wave functions now can be written as

$$\psi_1 = Ae^{ik_1 x} + \frac{k_1 - k_2}{k_1 + k_2} Ae^{-k_1 x} = \Psi_{inc} + \psi_{ref} \text{ for } x < 0$$

$$\psi_2 = \frac{2k_1}{k_1 + k_2} Ae^{ik_2 x} = \psi_{\text{trans}}, \quad \text{for } x > 0$$

3.3. POTENTIAL STEP OR SINGLE STEP BARRIER (E < V_0)

Let a particle of mass m and total energy E be incident from left (Region I) on the potential step

$$V(x) = V_0 \text{ at } x = 0, \text{ the origin of the } x\text{-axis.}$$

The potential energy of the particle is *zero* when it is to the left of the step *i.e.* left of the origin O and the potential energy $V(x) = V_0$ to the right of step or the origin.

$$\therefore \quad V(x) = 0 \text{ for } x < 0 \qquad \text{Region I}$$
$$= V_0 \text{ for } x \geq 0 \qquad \text{Region II}$$

Now as the total energy of the incident particle is less than V_0, the value of the step potential *i.e.* E < V_0, so $\sqrt{2m\,(\mathrm{E}-V_0)}$ is imaginary and classically the particle is reflected at $x = 0$ and it will not be able to penetrate the barrier because it does not possess sufficient energy to be in the region $x > 0$.

From *quantum mechanical view point*, the motion of the particle is governed by Schrödinger's wave equation for regions I and II. As the potential V_0 is independent of time, we have to solve Schordinger's time independent wave equation to analyse the behaviour of the particle. It is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\,(\mathrm{E} - V(x)]\;\psi = 0 \tag{3.38}$$

For region I. ($x < 0$), $V(x) = 0$. Let in this region ψ be denoted by ψ_1. Substituting $V(x) = 0$ is eqn (3.38), we have

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}\,\mathrm{E}\psi_1 = 0$$

Putting $\sqrt{\dfrac{2mE}{\hbar^2}} = k_1$ in the above equation, we have

$$\frac{d^2\psi_1}{dx^2} + k_1^2\,\psi_1 = 0 \tag{3.39}$$

The general solution of the eqn. (3.39) is given by

$$\psi_1 = \mathrm{A}e^{ik_1x} + \mathrm{B}e^{-ik_1x} \tag{3.40}$$

where A and B are arbitrary constants. The first-term $\mathrm{A}e^{ik_1x}$ represents the wave associated with the incident particle (incident wave) and the second term $\mathrm{B}e^{-ik_1x}$ is the reflected wave, which arises due to reflection at the potential step.

For region II. $(x > 0)$, $V(x) = V_0$. Let in this region ψ be denoted by ψ_2. Substituting $V(x) = V_0$ in eqn. (3.38), we have

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\,\psi_2 = 0 \tag{3.41}$$

In the present case, $E < V_0$, so $(E - V_0)$ is a negative quantity. Putting $(E - V_0) = -(V_0 - E)$, we have

$$\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\,\psi_2 = 0 \tag{3.42}$$

Substituting $\sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = k_2$ in the above equation, we have

$$\frac{d^2\psi_2}{dx^2} - k_2^2\,\psi_2 = 0 \tag{3.43}$$

The general solution of the equation is

$$\psi_2 = Ce^{-k_2x} + De^{k_2x} \tag{3.44}$$

where C and D are arbitrary constants. The wave function ψ_2 becomes infinite as $x \to \infty$ due to the presence of the term De^{k_2x} as this term increases indefinitely with x *i.e.* $e^{k_2x} \to \infty$ for $x \to +\infty$ making $\psi_2 \to \infty$. This violates the boundary conditions (as ψ_2 has to be finite everywhere). Hence we must have $D = 0$. Substituting $D = 0$ in eqn. (3.43), we get

$$\psi_2 = Ce^{-k_2x} \tag{3.45}$$

Definition of Constants

For evaluating B and C in terms of A, we apply the boundary conditions, which require that wave function and its derivative must be continuous at the boundary *i.e.* at $x = 0$ *i.e.*

$$\psi_1 = \psi_2 \qquad (\text{at } x = 0)$$

and

$$\frac{\partial\psi_1}{\partial x} = \frac{\partial\psi_2}{\partial x} \qquad (\text{at } x = 0)$$

Putting $x = 0$ in eqns (3.40) and (3.45) and equating $\psi_1 = \psi_2$, we get

$$A + B = C \tag{3.46}$$

Now differenting eqns (3.40) and (3.45) we have

$$\frac{\partial\psi_1}{\partial x} = ik_1(Ae^{ik_1x} - Be^{-ik_1x}) \tag{3.47}$$

and

$$\frac{\partial\psi_2}{\partial x} = -k_2Ce^{-k_2x} \tag{3.48}$$

Putting $x = 0$ in eqns. (3.47) and (3.48) and equating

$$\frac{\partial \psi_1}{\partial x} = \frac{\partial \psi_2}{\partial x} \text{ we have}$$

$$ik_1(A - B) = -k_2 C$$

$$A - B = \frac{-k_2}{ik_1} C = i\frac{k_2}{k_1} C \tag{3.49}$$

Adding eqns (3.46) and (3.49), we get

$$2A = C + i\frac{k_2}{k_1} C$$

$$C = \frac{2k_1}{k_1 + ik_2} A = \frac{2\,ik_1}{ik_1 - k_2} A \tag{3.50}$$

Subtracting eqn. (3.49) from (3.46), we get

$$2B = C - i\frac{k_2}{k_1} C = \left(\frac{k_1 - ik_2}{k_1}\right) C$$

$$= \left(\frac{ik_1 + k_2}{ik_1}\right) C = \frac{ik_1 + k_2}{ik_1} \times \frac{2\,ik_1}{ik_1 - k_2} A$$

$$= \left(\frac{ik_1 + k_2}{ik_1 - k_2}\right) 2A$$

or

$$B = \frac{ik_1 + k_2}{ik_1 - k_2} A \tag{3.51}$$

Thus wave functions (3.40) and (3.45) can be written as

$$\psi_1 = Ae^{ik_1x} + A\left(\frac{ik_1 + k_2}{ik_1 + k_2}\right) e^{-ik_1x} \qquad \text{for } x < 0$$

$$\psi_2 = A\,\frac{2\,ik_1}{ik_1 - k_2}\, e^{-k_2x} \qquad \text{for } x > 0$$

The probability current density for the transmitted wave will be

$$J_{\text{trans}} = \frac{\hbar}{2im}\left[\psi_2^* \frac{\partial \psi_2}{\partial x} - \psi_2 \frac{\partial \psi_2^*}{\partial x}\right]$$

$$= \frac{\hbar}{2im}\,[C^* e^{-kx} C(-k) e^{-kx} - Ce^{-kx} C^*(-k) e^{-kx}]$$

$$= \frac{\hbar}{2mi}\,[-CC^* k e^{-2kx} + CC^* k e^{-2kx}] = 0$$

$$\therefore \text{ Transmission probability, } |T|^2 = \frac{J_{\text{Trans}}}{J_{\text{inci}}} = \frac{0}{J_{\text{inci}}} = 0 \tag{3.52}$$

Also reflected current density in this case is

$$J_{\text{ref}} = Re\left[\frac{\hbar}{im} \psi^*_{\text{ref}} \frac{\partial \psi_{\text{ref}}}{\partial x}\right]$$

$$= \mathrm{Re}\left[\frac{\hbar}{im}\left(\frac{-ik+k_2}{-ik_1-k_2}\right)A^* e^{ik_1x}(-ik_1)\left(\frac{ik_1+k_2}{ik_1-k_2}\right)Ae^{-ik_1x}\right]$$

$$= \frac{-\hbar k_1}{m}|A|^2$$

Similarly

$$J_{inci} = \frac{+\hbar k_1}{m}|A|^2$$

$$\therefore \text{ Reflection probability, } |R|^2 = \frac{J_{ref}}{J_{inci}} = 1$$ (3.5[illegible])

Penetration (or Leakage) Through the Potential Barrier

From eqns (3.52) and (3.53), it is evident that the incident wave is totally reflected; there is no transmission. The fact that there is no transmission is also obvious from the fact that $J|_{x>0} = 0$ (or $J_{ref} = J_{inci}$ i.e. the whole of the J_{inci} is reflected back for $x < 0$) and the transmission probability vanishes but the wave function (eqn. (3.45)) is still not zero in the region to right of step ($x > 0$). It means that there is a finite probability of finding the particle in classically forbidden region $x > 0$. This phenomena is known as **quantum mechanical tunnelling** in which, although the region ($x > 0$) is classically forbidden for the particle but quantum mechanically, there is a finite probability (calculated as under) of appearance of the particle in the classically forbidden region ($x > 0$). The shape of wave amplitudes in the two regions is shown in Fig. 3.6.

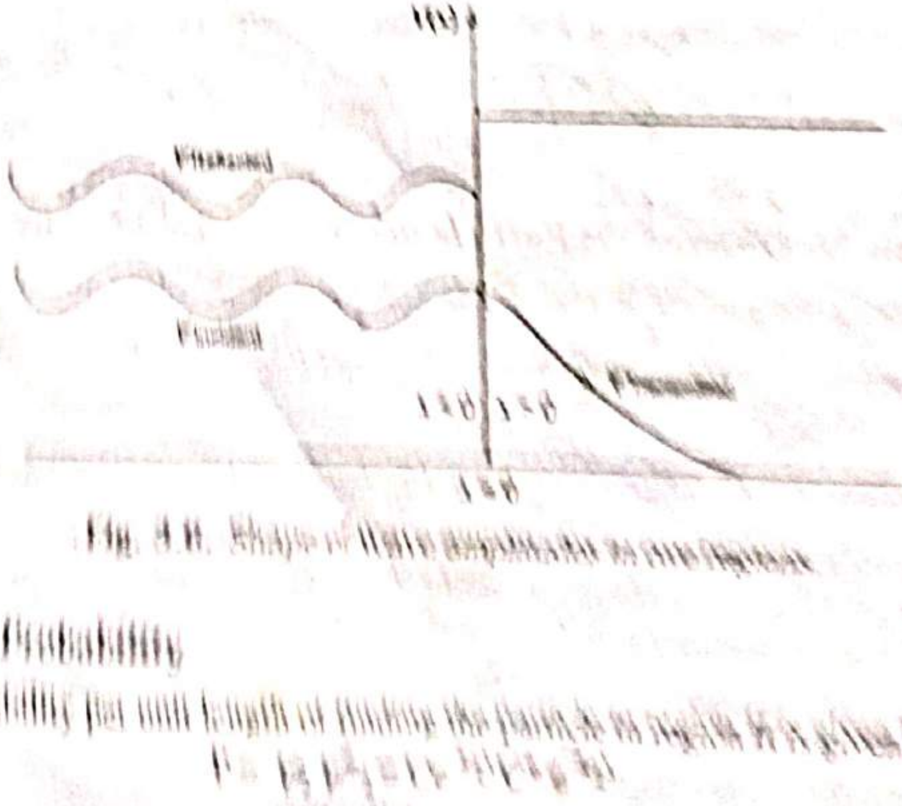

Fig. 3.6. Shape of wave amplitudes in two regions.

Leakage Probability

The probability per unit length of finding the particle in region II is given by

$$P = [illegible]$$

$$= [illegible]$$

Now
$$CC^* = A\frac{2ik_1}{ik_1 - k_2} \cdot A\frac{-2ik_1}{-ik_1 - k_2}$$

$$= A^2\frac{4k_1^2}{k_1^2 + k_2^2}$$

$$P = A^2\frac{4k_1^2}{k_1^2 + k_2^2}e^{-2k_2 x} \qquad (3.54)$$

Thus there is a finite probability of finding the particle in the region $x > 0$ or leakage. Eqn. (3.54) shows that probability of finding the particle in region II decreases exponentially with increasing x as shown in Fig. (3.6).

Penetration Depth

The penetration distance or depth of penetration is defined as the distance in which the wave function ψ_2 reduces to $1/e$ of its value at $x = 0$.

The wave function ψ_2 at $x = 0$, $Ce^{-k_2 x} = Ce^{-k_2 \times 0} = C$

Let Δx be the distance from $x = 0$, where the wave function is $1/e$ of its value at $x = 0$.

$$\boxed{\psi_2(x = \Delta x) = \frac{1}{e}\,\psi_2(x = 0)}$$

$$Ce^{-k_2\Delta x} = \frac{1}{e}C$$

$$e^{-k_2\Delta x} = \frac{1}{e} = e^{-1}$$

$$k_2\Delta x = 1$$

$$\Delta x = \frac{1}{k_2} = \frac{\hbar}{\sqrt{2m(V_0 - E)}} \qquad (3.55)$$

How Can We Observe the Particle in Classically Forbidden Region?

For observing the particle in region $x > 0$, it must be localized within a distance $\Delta x \approx \frac{1}{k}$ and its momentum must be uncertain by $\Delta p_x \geq \frac{\hbar}{\Delta x} \approx \hbar k = \sqrt{2m(V_0 - E)}$.

Thus uncertainty in K.E. $\approx \frac{(\Delta p_x)^2}{2m} \approx (V_0 - E)$. Hence its final energy which is E plus the added K.E. from localizing the particle is sufficient to raise it into the classically allowed region. In other words, if we try to observe the particle in the region $x > 0$, we necessarily impart so much of K.E. to it that the total energy is $> V_0$.

3.4. ONE DIMENSIONAL POTENTIAL BARRIER

Let us consider one dimensional potential barrier problem (Fig. 3.7) where the potential function is defined as

$$\left.\begin{aligned} V(x) &= 0 \text{ for } x < 0 \\ &= V_0 \text{ for } 0 < x < a \\ &= 0 \text{ for } x > a \end{aligned}\right\} \tag{3.56}$$

Here the potential barrier is between $x = 0$ and $x = a$ (*i.e.* width of the barrier = a)

From symmetry, it is clear that the particle (or wave) can be incident on the barrier either from the left or from the right. Let a particle having energy less than V_0 *i.e.* $E < V_0$ approach this barrier from the left *i.e.* from region I, then classically the particle will always be reflected and hence will not penetrate the barrier. However, quantum mechanically even for $E < V_0$, there is a finite probability of the particle penetrating through the barrier and appearing in the region III. This probability of penetrating the barrier is termed as the *tunnel effect*. This is entirely a quantum mechanical effect and the phenomena like field emission of electrons, emission of α-particles from the nucleus etc. are examples of this tunnelling effect. There is no classical analogue of this effect.

Further for $E > V_0$, classically, the particle will always get transmitted through the barrier, whereas quantum mechanically there is a finite probability that the particle will get reflected in region I and will penetrate the barrier and appear in region III.

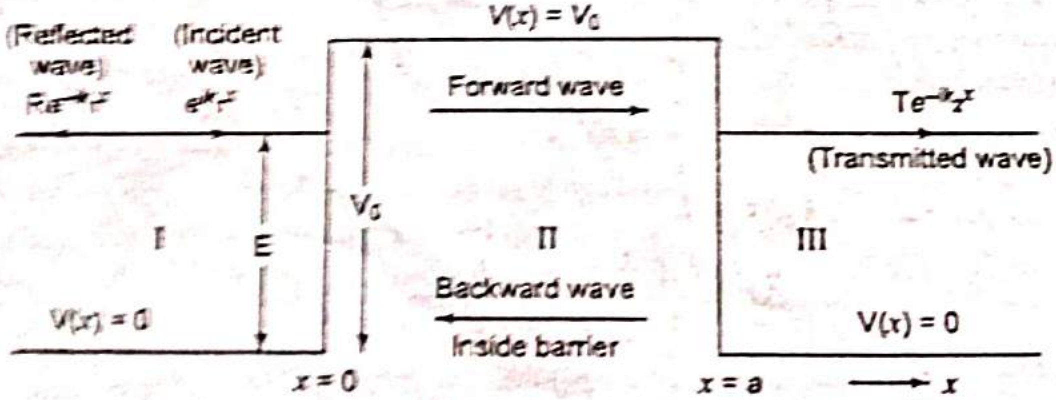

Fig. 3.7.

In order to solve this problem, let us write Schrondinger equation, in each of the three regions I, II and III (Fig. 3.7).

For region I *i.e.* for $x < 0$

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2} E\psi_1 = 0 \; [V(x) = 0] \tag{3.57}$$

For region II *i.e.* for $0 < x < a$

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_0)\psi_2 = 0 \; [V(x) = V_0] \tag{3.58}$$

For region III *i.e.* for $x > a$

$$\frac{d^2\psi_3}{dx^2}+\frac{2m}{\hbar^2}E\psi_3 = 0 \; [V(x)=0] \tag{3.59}$$

Here ψ_1, ψ_2, and ψ_3 are wave functions in regions I, II and III respectively. The general solutions of eqns of (3.57), (3.58) and (3.59) may be written as

$$\psi_1 = Ae^{ik_1x}+Be^{-ik_1x} \tag{3.60}$$

$$\psi_2 = Ce^{ik_2x}+De^{-ik_2x} \tag{3.61}$$

$$\psi_3 = Ee^{ik_1x}+Fe^{-ik_1x} \tag{3.62}$$

where A, B, C, D, E and F are constants, to be determined by using the usual boundary and continuity conditions on wave function and its gradient and

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \text{ and } k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \tag{3.63}$$

In eqn. (3.60), the first term represents the wave travelling along + ve x-axis in the region I *i.e.* the *incident wave* and the second term represents the wave reflected in region I at $x = 0$.

In eqn. (3.61), the first term represents the wave travelling along +ve x-direction in the region II. *i.e.* the wave transmitted at $x = 0$ and second term represents the wave travelling along –ve x-axis is region II. *i.e.* the wave reflected at $x = a$.

In eqn. (3.62), the first-term represents the wave travelling along +ve x-direction in the region III *i.e.* the wave transmitted at $x = a$, while the second term represents the wave travelling along –ve x-axis is region III; but there is no wave moving in the backward direction in region III (as there will be only waves moving in the forward direction in region III). Consequently, F = 0 so that the solution of eqn. (3.59) in region III *i.e.* eqn. (3.62) can be written as

$$\psi_3 = Ee^{ik_1x} \tag{3.64}$$

Now choosing the incident wave amplitude (A) as unity, we fix the constants B, C, D and E relative to unit amplitude A. Replacing B with R and E with T (*i.e.* R as reflection coefficient and T as transmission coefficient) respectively the solutions (3.60) and (3.64) are written as

$$\psi_1 = 1e^{ik_1x}+Re^{-ik_1x} \tag{3.65}$$

$$\psi_2 = Ce^{ik_2x}+De^{-ik_2x} \tag{3.66}$$

$$\psi_3 = Te^{ik_1x} \tag{3.67}$$

For evaluating R, C, D and T, boundary and continuity conditions on wave function and its gradient at the two boundaries $x = 0$ and $x = a$ are applied. These conditions are

(*a*) **Condition (i):** The ψ must be continuous at the boundaries *i.e.*

$$\psi_1 = \psi_2 \text{ at } x = 0 \text{ i.e. } \psi_1(0) = \psi_2(0) \tag{3.68(a)}$$

$$\psi_2 = \psi_3 \text{ at } x = a \text{ i.e. } \psi_2(a) = \psi_3(a) \tag{3.68(b)}$$

(*b*) **Condition (ii):** The $\frac{\partial\psi}{\partial x}$ must be continuous at the boundaries *i.e.*

$$\frac{\partial\psi_1}{\partial x} = \frac{\partial\psi_2}{\partial x} \text{ at } x = 0 \quad i.e. \quad \frac{\partial\psi_1(0)}{\partial x} = \frac{\partial\psi_2(0)}{\partial x} \tag{3.69(a)}$$

$$\frac{\partial \psi_2}{\partial x} = \frac{\partial \psi_3}{\partial x} \text{ at } x = a \quad i.e \quad \frac{\partial \psi_2(a)}{\partial x} = \frac{\partial \psi_3(a)}{\partial x} \tag{3.69(b)}$$

Applying condition (3.68(b)) to eqns. (3.65) and (3.66), we have

$$1 + R = C + D \tag{3.70}$$

Applying condition (3.68(b)) to eqns. (3.66) and (3.67), we have

$$Ce^{ik_2a} + De^{-ik_2a} = Te^{ik_1a} \tag{3.71}$$

Differentiating eqns (3.65) to (3.67), we get

$$\frac{\partial \psi_1}{\partial x} = ik_1 (e^{ik_1x} - Re^{-ik_1x}) \tag{3.72}$$

$$\frac{\partial \psi_2}{\partial x} = ik_2 (Ce^{ik_2x} - De^{-ik_2x}) \tag{3.73}$$

$$\frac{\partial \psi_3}{\partial x} = ik_1\, e^{ik_1x} \tag{3.74}$$

Applying boundary conditions (3.69a) and (3.69b) to these equations, we have

$$ik_1 (1 - R) = ik_2 (C - D) \tag{3.75}$$

$$ik_2 (Ce^{ik_2a} - De^{-ik_2a}) = ik_1\, Te^{ik_1a} \tag{3.76}$$

From eqns (3.70) and (3.75), we get

$$1 + R = C + D$$

$$1 - R = \frac{k_2}{k_1}(C - D)$$

Adding and subtracting these equations, we get

$$2C = (1 + R) + \frac{k_1}{k_2}(1 - R)$$

$$= \left(1 + \frac{k_1}{k_2}\right) + R\left(1 - \frac{k_1}{k_2}\right) \tag{3.77}$$

and

$$2D = (1 + R) - \frac{k_1}{k_2}(1 - R)$$

$$= \left(1 - \frac{k_1}{k_2}\right) + R\left(1 + \frac{k_1}{k_2}\right) \tag{3.78}$$

Similarly from eqns (3.71) and (3.76), we get

$$2\,Ce^{ik_2a} = Te^{ik_1a}\left(1 + \frac{k_1}{k_2}\right) \tag{3.79}$$

and

$$2\,De^{-ik_2a} = Te^{ik_1a}\left(1 - \frac{k_1}{k_2}\right) \tag{3.80}$$

Substituting for 2C from eqn. (3.77) in eqn. (3.79) and for 2D from eqn. (3.78) in eqn. (3.80), we get

$$\left\{\left(1+\frac{k_1}{k_2}\right)+R\left(1-\frac{k_1}{k_2}\right)\right\}e^{ik_2a}=Te^{ik_1a}\left(1+\frac{k_1}{k_2}\right) \tag{3.81}$$

and

$$\left\{\left(1-\frac{k_1}{k_2}\right)+R\left(1+\frac{k_1}{k_2}\right)\right\}e^{-ik_2a}=Te^{ik_1a}\left(1-\frac{k_1}{k_2}\right) \tag{3.82}$$

Dividing eqn. (3.81) by eqn.(3.82), we get

$$\frac{\left\{\left(1+\frac{k_1}{k_2}\right)+R\left(1-\frac{k_1}{k_2}\right)\right\}}{\left\{\left(1-\frac{k_1}{k_2}\right)+R\left(1+\frac{k_1}{k_2}\right)\right\}}=\frac{\left(1+\frac{k_1}{k_2}\right)}{\left(1-\frac{k_1}{k_2}\right)}$$

or

$$\left\{\left(1+\frac{k_1}{k_2}\right)\left(1-\frac{k_1}{k_2}\right)+R\left(1-\frac{k_1}{k_2}\right)^2\right\}e^{ik_2a}$$

$$=\left\{\left(1-\frac{k_1}{k_2}\right)\left(1+\frac{k_1}{k_2}\right)+R\left(1+\frac{k_1}{k_2}\right)^2\right\}e^{-ik_2a}$$

or

$$R\left\{\left(1-\frac{k_1}{k_2}\right)^2e^{ik_2a}-\left(1+\frac{k_1}{k_2}\right)^2e^{-ik_2a}\right\}$$

$$=\left(1-\frac{k_1}{k_2}\right)\left(1+\frac{k_1}{k_2}\right)\{e^{-ik_2a}-e^{ik_2a}\}$$

Putting $\frac{k_2}{k_1}=\overset{\mu}{\underline{m}}$, and expanding exponentials in terms of sine and cosine, we get

$$R\left\{\left(1-\frac{1}{\mu}\right)^2(\cos k_2a+i\sin k_2a)-\left(1+\frac{1}{\mu}\right)^2(\cos k_2a-i\sin k_2a)\right\}$$

$$=\left(1-\frac{1}{\mu^2}\right)(\cos k_2a-i\sin k_2a-\cos k_2a-i\sin k_2a)$$

or $R\,\{\cos k_2a\,[(\mu-1)^2-(\mu+1)^2]+i\sin k_2a\,[(\mu-1)^2+(\mu+1)^2]\}$

$$=-2i\,(\mu^2-1)\sin k_2a$$

or

$$R\,[-4\mu\times\cos k_2a+2i\sin k_2a\,(\mu^2+1)]=2i\,(1-\mu^2)\sin k_2a$$

$$R\,[\sin k_2a\,(\mu^2+1)+2\mu i\cos k_2a]=(1-\mu^2)\sin k_2a$$

or ***R (Reflection coeff in region I)*** $=\dfrac{(1-\mu^2)\sin k_2a}{(1+\mu^2)\sin k_2a+2i\,\mu\cos k_2a}$ (3.83)

Similarly, we get from eqn. (3.82)

$$Te^{ik_1a}\left(1-\frac{1}{\mu}\right)=\left\{\left(1-\frac{1}{\mu}\right)+R\left(1+\frac{1}{\mu}\right)\right\}e^{-ik_2a}$$

or

$$Te^{ik_1a}(\mu-1)=\left\{(\mu-1)+\frac{(1-\mu^2)\sin k_2a}{(1+\mu^2)\sin k_2a+2i\mu\cos k_2a}(\mu+1)\right\}e^{-ik_2a}$$

$$= \frac{\sin k_2a\left[(\mu-1)(1+\mu^2)+(1-\mu^2)(\mu+1)\right]+2i\mu(\mu-1)\cos k_2a}{(1+\mu^2)\sin k_2a+2i\,\mu\cos k_2a}\,e^{-ik_1a}$$

$$= \frac{-2\mu(\mu-1)\sin k_2a+2i\,\mu(\mu-1)\cos k_2a}{(1+\mu^2)\sin k_2a+2i\,\mu\cos k_2a}\,e^{-ik_1a}$$

$$= \frac{2i\,\mu(\mu-1)\{\cos k_2a+i\sin k_2a\}}{(1+\mu^2)\sin k_2a+2i\,\mu\cos k_2a}\,e^{-ik_1a}$$

$$= \frac{2i\,\mu(\mu-1)\,e^{ik_2a}\cdot e^{-ik_2a}}{(1+\mu^2)\sin k_2a+2i\,\mu\cos k_2a}$$

or T (*transmission coeff in region III*)

$$= \frac{2i\,\mu\,e^{-ik_1a}}{(1+\mu^2)\sin k_2a+2i\,\mu\cos k_2a} \tag{3.84}$$

The reflection and transmission coefficients are, in general, complex number as can be seen from eqns (3.83) and (3.84). Their amplitudes can be evaluated by taking modulus of these quantities *i.e.* $|R|$ and $|T|$ where $|R|^2$ and $|T|^2$ will represent the probability for reflection and transmission respectively

Now $$|R|^2 = R\times R^* = \left[\frac{(1-\mu^2)\sin k_2a}{2\mu i\cos k_2a+(1+\mu^2)\sin k_2a}\right]\times \left[\frac{(1-\mu^2)\sin k_2a}{-2\mu i\cos k_2a+(1+\mu^2)\sin k_2a}\right]$$

$$= \frac{(1-\mu^2)^2\sin^2 k_2a}{4\mu^2\cos^2 k_2a+(1+\mu^2)^2\sin^2 k_2a} \tag{3.85}$$

and $$|T|^2 = T\times T^* = \left[\frac{2\mu i e^{-ik_1a}}{(1+\mu^2)\sin k_2a+2\,i\,\mu\cos k_2a}\right]\times \left[\frac{-2\mu\,i\,e^{ik_1a}}{(1+\mu^2)\sin k_2a-2i\,\mu\cos k_2a}\right]$$

$$= \frac{4\mu^2}{(1+\mu^2)^2\sin^2 k_2a+4\mu^2\cos^2 k_2a} \tag{3.86}$$

The $|T|^2$ is an increasing function with E and its variation with E as a function of V_0 and a can be examined through the following special cases.

Special cases

1. When E approaches V_0 *i.e.* $E \to V_0$ (or $k_2 \to 0$)

Now $\mu = \frac{k_2}{k_1} = \sqrt{1-\frac{V_0}{E}} \to 0$ (for $E \to V_0$)

Let us evaluate $|T|^2$ in the limit $E \to V_0$ (or $k_2 \to 0$)

From eqn. (3.86), $$|T|^2 = \frac{4}{(1+\mu^2)^2 \frac{\sin^2 k_2 a}{\mu^2} + 4\cos^2 k_2 a}$$

$$= \frac{4}{(1+\mu^2)^2 \left(\frac{\sin k_2 a}{k_2 a}\right)^2 k_1^2 a^2 + 4\cos^2 k_2 a}$$

As $k_2 \to 0$, then $\mu \to 0$ and in this limit

$$|T|^2 = \frac{4}{k_1^2 a^2 + 4} = \frac{1}{1 + \frac{k_1^2 a^2}{4}}$$

(using $\frac{\sin k_2 a}{k_2 a} \to 1$ and $\cos k_2 a \to 1$ as k_2 or $k_2 a \to 0$)

$$= \frac{1}{1 + \left(\frac{k_1 a}{2}\right)^2} \qquad (3.87)$$

2. When $E > V_0$

Now $$|T|^2 = \frac{4\mu^2}{(1+\mu^2)^2 \sin^2 k_2 a + 4\mu^2 \cos^2 k_2 a}$$

Here $$\mu = \sqrt{1 - \frac{V_0}{E}}$$

will be real and positive for $E > V_0$ and its value is less than one (*i.e.* $\mu < 1$)

Let us find the condition for perfect transmission for which

$$|T|^2 = 1$$

This will correspond to

$$(1+\mu^2)^2 \sin^2 k_2 a + 4\mu^2 \cos^2 k_2 a = 4\mu^2 \qquad \text{(from eqn. 2.86)}$$

or $$(1+\mu^2)^2 \sin^2 k_2 a + 4\mu^2 (1 - \sin^2 k_2 a) = 4\mu^2$$

or $$\{(1+\mu^2)^2 - 4\mu^2\} \sin^2 k_2 \alpha = 0$$

or $$(1-\mu^2)^2 \sin^2 k_2 a = 0$$

As $\mu < 1$, so $(1-\mu^2)^2$ cannot be zero

Hence $$\sin^2 k_2 a = 0$$

or $$\sin k_2 a = 0$$

or $$k_2 a = n\pi \qquad (3.88)$$

or $$\frac{2\pi}{\lambda} a = n\pi$$

or $$a = \frac{n\lambda}{2} \qquad (3.89)$$

Thus perfect transmission occurs when $a = \frac{n\lambda}{2}$, *i.e.* whenever barrier width a is an integral multiple of half wavelength.

This condition (*i.e.* eqn. (3.88)) can be expressed in terms of E and V_0

Now $$k_2 a = n\pi \text{ or } k_2 = \frac{n\pi}{a}$$

or $$\sqrt{\frac{2m(E - V_0)}{\hbar^2}} = \frac{n\pi}{a}$$

or $$(E - V_0) = \frac{n^2\pi^2}{a^2}\frac{\hbar^2}{2m}$$

or $$E = V_0\left(1 + \frac{n^2\pi^2\hbar^2}{V_0 2ma^2}\right) \tag{3.90}$$

Whenever eqn. (3.90) is satisfied in E and V_0, the perfect transmission will occur

if $$E \to \infty, \mu = \sqrt{1 - \frac{V_0}{E}} \to 1$$

and in this case

$$|T|^2 \to \frac{4}{4\sin^2 k_2 a + 4\cos^2 k_2 a} = \frac{4}{4(\sin^2 k_2 a + \cos^2 k_2 a)}$$

$$\therefore \quad |T|^2 \to 1$$

The phenomenon of penetration of a particle through a potential barrier of finite width and height is due to wave nature of matter and is called wave mechanical (quantum mechanical) tunnelling. α decay is the best known example of barrier penetration. Another prominent example of tunnelling is field emission tunnel diode. $|T|^2$ (eqn. 3.86) increases steadily with the energy of the incident particle for $E \geq V_0$ and attains a maximum value for the condition $E = V_0\left(1 + \frac{n^2\pi^2\hbar^2}{2ma^2 V_0}\right)$, after which its value oscillates slightly (or shows periodic variations) with maximum $|T|^2 = 1$, becoming asymptotically equal to unity for values of E that are very large compared to V_0 as shown in Fig. 3.8.

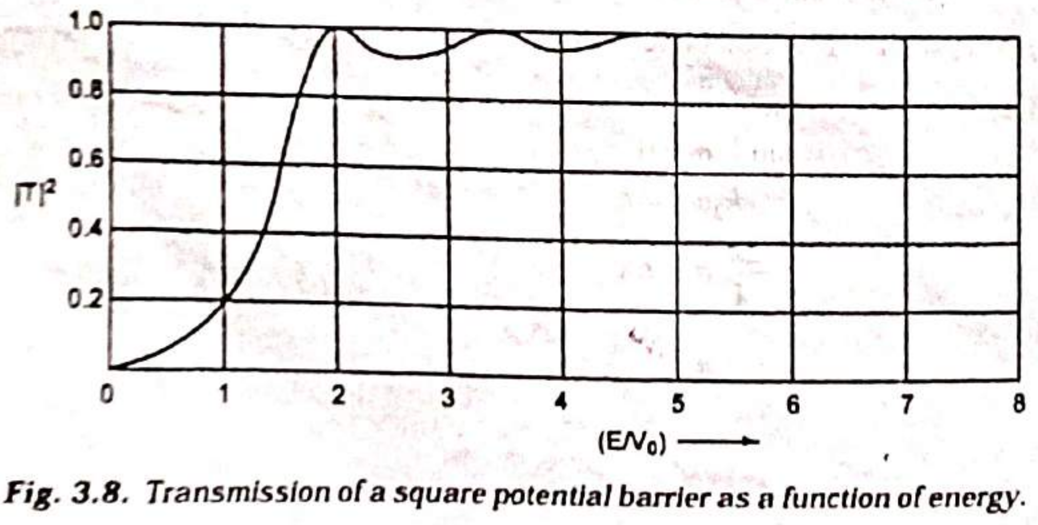

Fig. 3.8. Transmission of a square potential barrier as a function of energy.

In case of the [illegible] perfect transmission [illegible] certain wave-length [illegible] interference is [illegible]

1. When $E < V_0$, k_2 is purely imaginary and

$$k_2 = \sqrt{[illegible]} = [illegible]$$

$= ik$, where k is real and positive quantity

Now $$|T|^2 = \frac{4k_1^2 k_2^2}{\left(1 - \frac{k_2^2}{k_1^2}\right)^2 \sin^2 k_2 a + \frac{4k_2^2}{k_1^2} \cos^2 k_2 a}$$ [illegible]

Putting $k_2 = ik$, we get

$$|T|^2 = \frac{-4k_1^2 k^2}{\left(1 - \frac{k^2}{k_1^2}\right)^2 i^2 \sinh^2 ka - \frac{4k^2}{k_1^2} \cosh^2 ka}$$

where $\sin(i\theta) = i \sinh\theta$ and $\cos(i\theta) = \cosh\theta$

or $$|T|^2 = \frac{4k_1^2 k^2}{\left(1 - \frac{k^2}{k_1^2}\right)^2 \sinh^2 ka + \frac{4k^2}{k_1^2} \cosh^2 ka}$$

or $$|T|^2 = \frac{4k_1^2 k^2}{(k_1^2 - k^2) \sinh^2 ka + 4k^2 k_1^2 \cosh^2 ka} \quad [illegible]$$

which is positive and less than unity. For $E = 0$ or ($k_1 = 0$) we $|T|^2 = 0$. It means that $|T|^2$ is zero for $E = 0$ and as E increases ($\le V_0$), $|T|^2$ also increases smoothly and [illegible] smoothly the value (3.87) for $E = V_0$ and attains the maximum value as discussed earlier and also shown in Fig. 2.8.