Kunthavai Naachiyaar Goverment Arts College for Women, Thanjavur.

Department of Physics

WAVE MECHANICS AND NUCLEAR PHYSICS

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Wave Mechanics

Unit_I Dual nature of matter

7.1 Introduction

According to de Broglie a moving particle, whatever its nature, has wave properties associated with it. He proposed that the wavelength λ associated with any moving particle of momentum p (mass m and velocity v) is given by

 $(\lambda = \frac{h}{p} = \frac{h}{mv}, \qquad ... (1)$ where h is Planck's constant. Such waves associated with the matter particles are called matter waves or de Broglie waves Bohr's Theory of the hydrogen atom led de Broglie to the conception of matter waves. According to Bohr's theory, the stable states of electrons in the atom are governed by "integer rules". The only phenomena involving integers in Physics are those of interference and modes of vibration of stretched strings, both of which imply wave motion. Hence de Broglie thought that the electrons may also be characterised by a periodicity. So he proposed that matter, like radiation, has dual nature. Eq. (1) was verified by experiments involving the diffraction of electrons by crystals.

The de Broglie Wavelength

A photon of light of frequency v has the momentum

$$p = hv/c$$

But $v = c/\lambda$. Therefore, the momentum of the photon can be expressed in terms of wavelength λ as

$$p = h/\lambda$$
.

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

$$\lambda = h/p \qquad \dots (1)$$

de Broglie suggested that Eq.(1) is a completely general one that applies to material particles as well as to photons. The momentum of a particle of mass m and velocity v is p = mv, and its de Broglie wavelength is accordingly

 $\lambda = h/mv$

If E_k is the kinetic energy of the material particle, then

$$p = \sqrt{(2m E_k)}$$

Therefore, de Broglie wavelength of particle of K.E. = E_k is given by

$$\lambda = \frac{h}{\sqrt{2m}E_k} \qquad \dots (2)$$

If a charged particle carrying charge q is accelerated through a potential difference V volts, then kinetic energy $E_k = q V$.

:. The de Broglie wavelength for charged particle of charge q and accelerated through a potential difference of V volts is

$$\lambda = \frac{h}{\sqrt{2m \ qV}} \qquad \dots (3)$$

Example 1. Find the de Broglie wavelength associated with

- (i) A 46 gm golf ball with velocity 36 m/s.
- (ii) an electron with a velocity 10^7 m/s.

Which of these two show wave character and why? (Garhwal 1994)

Sol. (i) Since $v \ll c$, we can take $m = m_0 \rightarrow$ the rest mass. Hence

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34} \text{ J.s}}{(0.046 \text{ kg}) (36\text{m/s})}$$
$$= 4.0 \times 10^{-34} \text{ m.}$$

Thus the wavelength associated with golf ball is much smaller as compared to its dimensions. Hence no wave aspects can be expected in its behaviour.

(ii) Again $v \ll c$, so $m = m_0 = 9.1 \times 10^{-31}$ kg.

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{(9.1 \times 10^{-31}) \times 10^7} = 7.3 \times 10^{-11} \text{m}$$

This wavelength is comparable with the atomic dimensions. Hence a moving electron exhibits a wave character.

Example 2. Show that the de Broglie wavelength associated with an electron of energy V electron-volts is approximately $(1.227 / \sqrt{V})$ nm.

Sol. The de Broglie wavelength λ associated with an electron of mass m and energy E is given by

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

Here, kinetic energy $E_k = V \text{ eV} = 1.6 \times 10^{-19} \text{ VJ}$

$$\lambda = \frac{6.62 \times 10^{-34}}{\sqrt{(2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} V)}}$$
$$= \frac{1.227 \times 10^{-9} \text{m}}{\sqrt{V}} = \frac{1.227}{\sqrt{V}} \text{nm}$$

Example 3 Find the kinetic energy of a proton whose de Broglie wavelength is 1 fm.

Sol.
$$pc = (mv)c = hc/\lambda$$

$$\frac{(4.136 \times 10^{-15} \text{ eV.s})(3 \times 10^8 \text{ ms}^{-1})}{1 \times 10^{-15} \text{m}} = 1.241 \text{GeV}.$$

Rest energy of proton = $E_0 = 0.938 \text{ GeV}$.

 $pc > E_0$. Hence a relativistic calculation is needed.

The total energy of the proton is

$$E = \sqrt{E_0^2 + p^2 c^2} = \sqrt{(0.938 \text{GeV})^2 + (1.241 \text{GeV})^2} = 1.556 \text{ GeV}.$$

The kinetic energy of the proton is

$$KE = E - E_0 = (1.556 - 0.938) \text{ GeV} = 0.618 \text{ GeV}$$

Example 4. Show that the de Broglie wavelength for a material particle of rest mass m_0 and charge q, accelerated from rest through a potential difference of V volts relativistically is given by

$$\lambda = \frac{h}{\sqrt{2m_0qV\left(1 + \frac{qV}{2m_0c^2}\right)}}$$

Solution. We use the relativistic formula to find momentum.

Kinetic energy $E_k = aV$. $E^2 = p^2 c^2 + m_0^2 c^4$, $E = E_k + m_0 c^2 = qV + m_0 c^2$. So, $p^2 c^2 = E^2 - m_0^{-2} c^4 = (qV + m_0 c^2)^2 - m_0^2 c^4 = q^2 V^2 + 2m_0 c^2 qV$ $p^2 = 2m_0 qV \left(1 + \frac{qV}{2m_0 c^2}\right)$ or $p = \sqrt{2m_0 qV \left(1 + \frac{qV}{2m_0 c^2}\right)}$ $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m_0 qV \left(1 + \frac{qV}{2m_0 c^2}\right)}}$

Special Case. If the charged particle is an electron, then $q = e = 1.6 \times 10^{-19}$ C, $m_0 = 9.1 \times 10^{-31}$ kg.

$$\lambda = \frac{6.62 \times 10^{-34}}{\sqrt{(2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \text{ V}) \left(1 + \frac{1.6 \times 10^{-19} \text{ V}}{2 \times 9.1 \times 10^{-31} \times (3 \times 10^8)^2}\right)}}$$
$$= \frac{1.227}{\sqrt{V}} \times \frac{1}{\sqrt{1 + 9.768 \times 10^{-7} V}} \text{ nm}$$

Phase velocity (or Wave Velocity) of de Broglie Waves

A particle of mass m moving with velocity v has a wave associated with it whose wavelength is given by

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

Let E be the total energy of the particle. Let v be the frequency of the

associated wave. We equate the quantum expression E=hv with the relativistic formula for total energy $E=mc^2$. So we get

$$hv = mc^2$$
 or $v = mc^2/h$.

Let v_p be the de Broglie wave velocity. Then,

$$v_p = v\lambda = \left(\frac{mc^2}{h}\right) \left(\frac{h}{mv}\right) = \frac{c^2}{v}$$

But the particle velocity v is always less than c (the velocity of light). Therefore, the de Broglie wave velocity v_n must be greater than c.

7.2. Expression for Group Velocity

Consider two waves that have the same amplitude A but differ by an amount $\Delta \omega$ in angular frequency and an amount Δk in wave number. They can be represented by the equations

$$y_1 = A \cos (\omega t - kx)$$

$$y_2 = A \cos [(\omega + \Delta \omega) t - (k + \Delta k) x]$$

The superposition of the two waves will yield a single wave packet or wave group. Let us find the velocity v_g with which the wave group travels.

The resultant displacement y at any time t and any position x is the sum of y_1 and y_2 .

$$y = y_1 + y_2$$

$$= A \cos(\omega t - kx) + A \cos[(\omega + \Delta \omega) t - (k + \Delta k) x]$$

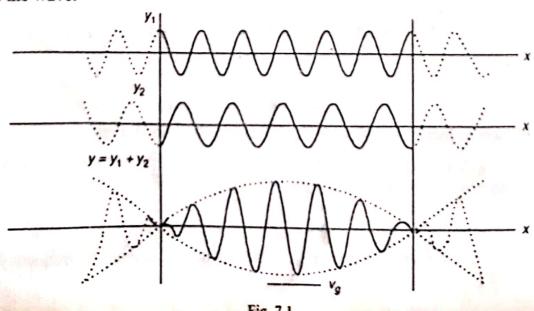
$$= 2 A \cos \frac{1}{2} [(2\omega + \Delta \omega) t - (2k + \Delta k) x] \cos \frac{1}{2} (\Delta \omega t - \Delta kx)$$

 $\Delta \omega$ and Δk are small compared with ω and k respectively. Therefore, $2\omega + \Delta \omega \approx 2\omega$

$$2k + \Delta k \approx 2k$$

$$y = 2A\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)\cos(\omega t - kx) \qquad ... (1)$$

This is the analytical expression for resultant wave (wave packet) due to superposition of the two waves. The second cosine function is the original wave. The coefficient of this cosine can be considered to be an amplitude that varies with x and t. This variation of amplitude is called the modulation of the wave.



Hence Eq. (1) represents a wave of angular frequency to and wave number k that has superimposed upon it a modulation of anuglar frequency $\frac{1}{2}\Delta\omega$ (Fig.7.1).

$$v_g = \frac{\Delta \omega}{\Delta k}$$
 ... (2)

The velocity v_g of the wave groups is $v_g = \frac{\Delta \omega}{\Delta k} \qquad ... (2)$ When ω and k have continuous spreads, the group velocity is given by $v_g = \frac{d\omega}{dk} \qquad ... (3)$

$$v_g = \frac{d\omega}{dk} \qquad ... (3)$$

This is the expression for the group velocity.

Group Velocity of de Broglie Waves

A particle moving with a velocity v is supposed to consist of a group of waves, according to de Broglie hypothesis.

The group velocity is given by,

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

The angular frequency and wave number of the de Broglie waves associated with a particle of rest mass m_0 moving with the velocity v are given by

$$\omega = 2 \pi v = \frac{2 \pi mc^2}{h} = \frac{2 \pi m_0 c^2}{h \sqrt{1 - v^2/c^2}}$$
 (1)

and

$$k = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h} = \frac{2\pi m v}{h\sqrt{1 - v^2/c^2}}$$
 ...(2)

By differentiation, we obtain

$$\frac{d\omega}{dv} = \frac{2\pi m_0 v}{h(1 - v^2/c^2)^{3/2}}$$
$$\frac{dk}{dv} = \frac{2\pi m_0}{h(1 - v^2/c^2)^{3/2}}$$

 $\frac{dk}{dv} = \frac{2 \pi m_0}{h(1 - v^2/c^2)^{3/2}}$ The group velocity v_g of the de Brolie waves associated with particle is

$$v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv} = v$$

Hence the de Broglie wave group associated with a moving particle travels with the same velocity as the particle.

Relation between Group Velocity (vg)and Wave Velocity or Phase Velocity (v_p)

We have the relations,

Wave velocity,
$$v_p = \frac{\omega}{k}$$
 ... (1)

Group velocity,
$$v_g = \frac{d\omega}{k}$$
 ... (2)

The wave number is given by

$$k=\frac{2\,\pi}{\lambda}$$

Also
$$\frac{dk}{d\lambda} = \frac{2\pi}{\lambda^2}$$

$$\omega = 2\pi v = 2\pi \frac{v_p}{\lambda}$$

$$\frac{d\omega}{d\lambda} = 2\pi \left[-\frac{v_p}{\lambda^2} + \frac{1}{\lambda} \frac{dv_p}{d\lambda} \right]$$
or
$$\frac{d\omega}{d\lambda} = -\frac{2\pi}{\lambda^2} \left[v_p - \lambda \frac{dv_p}{d\lambda} \right]$$

Dividing Eq. (4) by Eq. (3), we get

$$\frac{d\omega}{d\lambda} \cdot \frac{d\lambda}{dk} = \frac{-\frac{2\pi}{\lambda^2} \left[v_p - \lambda \frac{dv_p}{d\lambda} \right]}{-\frac{2\pi}{\lambda^2}}$$

$$\frac{d\omega}{dk} = v_p - \lambda \frac{dv_p}{d\lambda}$$

or
$$\frac{dk}{dk} = v_p - \lambda \frac{dv_p}{d\lambda}$$

$$\therefore \qquad v_g = v_p - \lambda \frac{dv_p}{d\lambda} \qquad (5)$$

Eq. (5) gives the relationship between group velocity (v_g) and phase velocity or wave velocity (v_p) .

From this equation the following two cases arise.

(i) For dispersive medium

 $v_p = f(\lambda)$. Usually $dv_p / d\lambda$ is positive (normal dispersion).

$$v_g < v_p$$
.

This is the case with de Broglie waves.

(ii) For non-dispersive medium

$$v_p \neq f(\lambda)$$
. $\frac{dv_p}{dt} = 0$. $v_g = v_p$
This result is true for electromagnetic waves in vacuum.

7.3 Experimental study of matter waves

Davisson and Germer's experiment.

Experimental arrangement. The experimental arrangement is shown in Fig. 7.2. Electrons are produced by heating a filament (F) by a low tension battery (L.T). These electrons are restricted to a fine parallel pencil by thin aluminium diaphragms D_1 and D_2 . The electrons are then accelerated by passing them through an aluminium cylinder A to which required high potentials (H.T) can be applied. This electron beam falls on a large single crystal of nickel NJThe crystal is capable of rotation about an axis parallel to the axis of the incident beam by a handle H. The electrons are scattered in all directions by the atoms in the crystal. The electrons scattered in different directions are collected by a Faraday cylinder C, called the collector. The collector is connected to a sensitive galvanometer G and can be

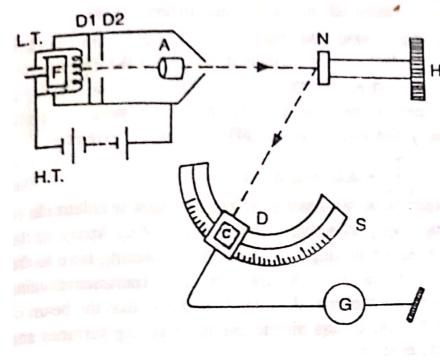
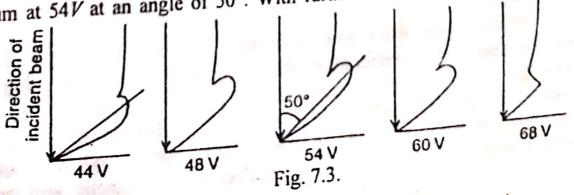


Fig. 7.2.

moved along a graduated circular scale S. so that it is able to rereflected the electrons at all angles between 20° and 90°. The collector has two walls C and D, insulated from each other. A retarding potential is applied between the two walls of collector so that only the electrons with nearly the incident velocity and secondary the not electrons, slow

longs to the face centred cubic type and it is so cut as to present a smooth reflecting surface parallel to the lattice plane (1 1 1). By turning the handle, any azimuth of the crystal can be presented to the plane defined by the incident beam and the reflected beam entering the collector.

electrons falls normally on the surface of the crystal. A diffraction effect from the surface layer of the crystal acting as a plane grating is produced. Fro each azimuth of the crystal, a beam of electrons is made to fall normally on the crystal. The collector is moved to various positions on the scale S and the galvanometer deflection at each position is noted. This deflection gives a measure of the intensity of the diffracted beam of electrons. The galvanometer deflection is plotted against the angle between the incident beam and the beam entering the collector (colatitude). The observations are repeated for different accelerating voltages and a number of curves are drawn (Fig. 7.3). The graph remains fairly smooth, till the accelerating voltage becomes 44 V when a spur appears on the curve. As the accelerating voltage is increased, the length of the spur increases, till it reaches a maximum at 54V at an angle of 50°. With further increases in the accelerating mum at 54V at an angle of 50°.



voltage, the spur decreases in length and finally disappears at 68 V.

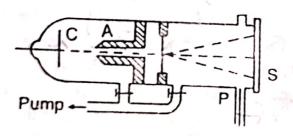
The occurrence of a pronounced spur ("bump") at 50° with the electrons accelerated through 54V can be explained, as due to the constructive interference of the electron waves, scattered in this direction, from the regularly spaced parallel planes in the crystal, which are rich in atoms. According to de Broglie's theory, the wavelength of 54V electrons is given by

$$\lambda = \frac{12.25}{\sqrt{.54}} A.U. = 1.66 A.U.$$

According to experiment, we have a diffracted beam at colatitude of 50°. For nickel, for the (1 1 1) reflecting plane, d = 2.15 A.U. Applying the equation for a plane reflection grating $n\lambda = d \sin \theta$, n referring here to the first order, we get, $\lambda = 2.15 \sin 50^{\circ} = 1.65$ A.U. Thus the experimental value is in close agreement with the theoretical value. This shows that the beam of electrons behaves like X-rays, suffers diffraction at reflecting surfaces and thus has wavelike characteristics.

G.P. Thomson's Experiment

Experimental arrangement. The experimental arrangement is shown in Fig. 7.4 (i). A beam of cathode rays is produced in a discharge tube AC by means of an induction coil. The electrons passing through a fine



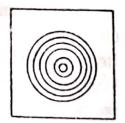


Fig. 7.4 (i)

Fig. 7.4 (ii)

hole A, are incident on a thin gold foil F. The thickness of the foil is about 10^{-8} m. The emergent beam of electrons is received on a photographic plate P. Visual examination of the pattern is made possible by the fluorescent screen S. A very high vacuum is maintained in the camera part FP of the apparatus while air is allowed to leak into the discharge tube section through a needle valve. Thus a beam of required voltage can be continuously produced, the discharge tube being sufficiently soft.

Experimental procedure. A beam of electrons of known velocity is made to fall on the photographic plate, after traversing the thin gold foil. When the plate is developed a symmetrical pattern consisting of concentric rings about a central spot, is obtained (Fig. 7.4 (ii)). This pattern is similar to the pattern produced by X-rays in the powdered crystal method. When the cathode rays in the discharge tube are deflected by a magnetic field, the en-

Scanned with CamScanner

tire pattern on the screen S is found to shift correspondingly. Thus the pattern is confirmed as due to diffracted electrons and not due to secondary X-rays, generated by the electrons going through the foil. Further, on removing the film F the pattern disappears, showing that the presence of the film is essential. If the electrons behaved as corpuscles, the electrons passing through the foil should have been scattered through a wide angle. Clearly, this experiment demonstrates that the electron beam behaves as waves, since diffraction patterns can be produced only by waves.

Verification of the de Broglie equation. G.P. Thomson employed very high voltages of the order of 50000 volts to accelerate the electrons. With very high speed electrons, relativistic correction for the mass of the electron has to be applied. It can be shown that

$$\lambda = \frac{12.27}{\sqrt{V}} \frac{1}{\sqrt{1 + 9.836 \times 10^{-7} V}} A.U. \tag{3}$$

The correction factor is very small, except for very large values of V.

To calculate λ from the radii of the rings. In the polycrystalline film there will be some crystals set at the correct angle to give a Bragg re-

flection. If there are enough crystals distributed at random, the result of such reflections will be a series of rings, arising from the intersection of the cones of diffraction with the photographic plate. Let AB be the incident beam passing though the film at B. BP is the direction of the beam which has suffered a Bragg reflection

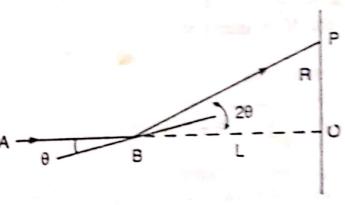


Fig. 7.5.

in some crystal in the film at B. This reflected beam falls at the point P on the photographic plate at a distance R from the central point O (Fig. 7.5). Let the distance BO, from the film to the plate, be L. $\angle PBO = 2\theta$ where θ is the glancing angle given by the Bragg relation,

$$n\lambda = 2d \sin \theta$$
.
 $R/L = \tan 2\theta = 2\theta$, since θ is small.

$$\therefore \qquad \theta = R/2L$$
But $2d \sin \theta = 2d\theta = n\lambda$ or $\theta = n\lambda/2d$

$$\therefore \qquad \frac{n\lambda}{2d} = \frac{R}{2L} \text{ or } \lambda = \frac{Rd}{nL}$$

From this the wavelength is calculated. This agrees with the calculated value given by Eqn. (1). This provides ultimate confirmation for the wave nature of the electron.

Example 1. 10 kV electrons are passed through a thin film of a metal for which the atomic spacing is 5.5×10^{-11} m. What is the angle of deviation of the first order diffraction maximum?

Wavelength of the electron =
$$\lambda = \frac{h}{\sqrt{2mVe}}$$

$$\therefore \qquad \lambda = \frac{6.626 \times 10^{-10}}{\sqrt{2(9.11 \times 10^{-31}) 10^4 (1.602 \times 10^{-19})}}$$
= 1.227 × 10⁻¹¹ m.

Applying Bragg's formula for diffraction at the atomic planes, $n\lambda = 2d \sin \theta$ or $1 \times (1.227 \times 10^{-11}) = 2 \times (5.5 \times 10^{-11}) \sin \theta$ or $\sin \theta = 0.1115$. $\therefore \theta = 6^{\circ}24'$.

Angle through which electron is deviated $= 2\theta = 12^{\circ}48'$

Two slit interference pattern with electrons

The interference of electron waves can be exhibited by a *double slit ex*periment. The interference pattern so obtained resembles the pattern in case of visible light and proves the association of wave-packets with electrons.

The experimental arrangement is shown in Fig. 7.6.

The electron gun (G) supplies a mono-energetic beam of electrons. The electrons emerging from the gun are allowed to pass through two slits

 S_1 and S_2 . The interference pattern is observed on a photographic film P. The entire apparatus is enclosed in a high vacuum chamber, so that electrons emerging from the gun travel to the screen without collisions in the path. When photographic film is observed with an electron microscope, it is observed that

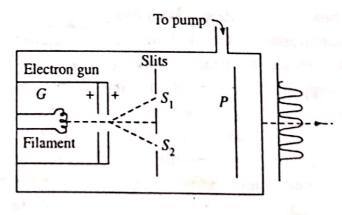


Fig. 7.6

interference fringes are obtained on the film. The distribution of intensity on the film is shown on the right. The formation of interference fringes clearly indicates the wave nature of electrons.

Knowing the separation between S_1 , S_2 and the distance between the plane of S_1 , S_2 and the photographic plate P, the value of wavelength associated with electrons may be calculated. This value comes out to be same as given by de-Broglie relation.

7.4. Heisenberg's uncertainty Principle

Statement. It is impossible to determine precisely and simultaneously the values of both the members of a pair of physical variables which

describe the motion of an atomic system. Such pairs of variables are called canonically conjugate variables.

According to this principle, the position and momentum Example. of a particle (say electron) cannot be determined simultaneously to any desired degree of accuracy.

Taking Δx as the error in determining its position and Δp the error in determining its momentum at the same instant, these quantities are related as follows:

$$\Delta x \Delta p = h/2\pi$$

The product of the two errors is approximately of the order of Planck's constant. If Δx is small, Δp will be large and vice versa. It means that if one quantity is measured accurately, the other quantity becomes less accurate. Thus any instrument cannot measure the quantities more accurately than predicted by Hgeisenberg's principle of uncertainty or indeterminacy. The same relation holds for the energy and time related to any given event.

i.e.,
$$\Delta E \Delta t = h/2\pi$$

According to classical ideas, it is possible for a particle to occupy a fixed position and have a definite momentum and we can predict exactly its position and momentum at any time later. But according to the uncertainty principle, it is not possible to determine accurately the simultaneous values of position and momentum of a particle at any time. Heisenberg's principle implies that in physical measurements probability takes the place of exactness and as such phenomena which are impossible according to classical ideas may find a small but finite probability of occurrence.

Illustration (i): Determination of position with a γ-ray microscope Suppose we try to measure the position and linear momentum of an electron

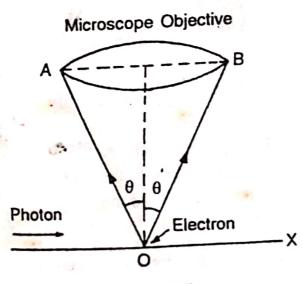


Fig. 7.7.

using an imaginary microscope with a very high resolving power (Fig. 7.7). The electron can be observed if atleast one photon is scattered by it into the microscope lens. The resolving power of the microscope is given by the relation

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

where Δx is the distance between two points which can be just resolved by microscope. This is the range in which the electron would be visible when disturbed by the photon. Hence Δx is the

uncertainty involved in the position measurement of the electron.

However, the incoming photon will interact with the electron through the Compton effect. To be able to see this electron, the scattered photon

should enter the microscope within the angle 20. The momentum imparted by the photon to the electron during the impact is of the order of h/λ . The component of this momentum along OA is $-\frac{h}{\lambda} \sin \theta$ and that along OB is $\frac{h}{\lambda} \sin \theta$. Hence the uncertainty in the momentum measurement in the x-direction is

 $\Delta p_x = \frac{h}{\lambda \lambda} \sin \theta - \frac{1}{\lambda} \left(-\frac{h}{\lambda} \sin \theta \right) = \frac{2h}{\lambda} \sin \theta.$ $\Delta x \times \Delta p_x = \frac{h}{2 \sin \theta} \times \frac{1}{\lambda} \sin \theta = h.$

A more sophisticated approach will show that $\Delta x \Delta p_x \ge h/2\pi$.

It is clear that the process of measurement itself perturbs the particle whose properties are being measured.

Illustration (ii): Diffraction of a beam of electrons by a slit.

A beam of electrons is transmitted through a slit and received on a photo-

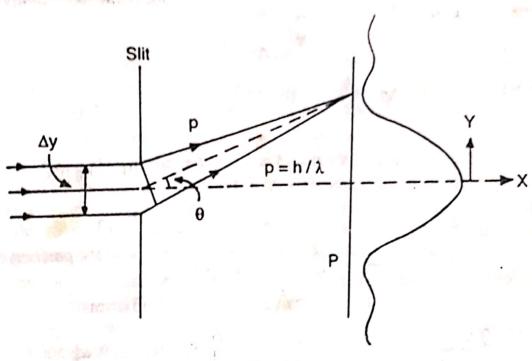


Fig. 7.8.

graphic plate P, kept at some distance from the slit (Fig. 7.8). We can only say that the electron must have passed through the slit and cannot specify its exact location in the slit as the electron crosses it. Hence the position of any electron recorded on the plate is uncertain by an amount equal to the width of the slit (Δy) . At λ be the wavelength of the electrons and θ be the angle of deviation corresponding to first minimum. From the theory of

diffraction in optics, $\Delta y = \frac{\lambda}{\sin \theta}$. This is the uncertainty in determining the position of electron along y-axis.

Initially the electrons are moving along X-axis and so they have no component of momentum along y-axis. As the electrons are deviated at the slit from their initial path to form the pattern, they acquire an additional

component of momentum along y-axis. If p is the momentum of the electron on emerging from the slit, the component of momentum of electron along y-axis is $p \sin \theta$. As the electron may be anywhere within the pattern from angle $-\theta$ to $+\theta$, the y-component of momentum of the electron may be anywhere between $-p \sin \theta$ and $+p \sin \theta$. Therefore, the uncertainty in the y-component of momentum of the electron

$$\Delta p_y = 2p \sin \theta = \frac{2h}{\lambda} \sin \theta$$
 $\left(\text{since } \lambda = \frac{h}{p} \right)$

$$\Delta y \, \Delta p_y = \frac{\lambda}{\sin \theta} \times \frac{2h}{\lambda} \sin \theta = 2h.$$

i.e., $\Delta y \Delta p_y \ge h/2\pi$, which is Heisenberg's uncertainty principle.

Example 1. A microscope, using photons, is employed to locate an electron in an atom to within a distance of 0.2 Å. What is the uncertainty in the momentum of the electron located in this way?

Here,
$$\Delta x = 0.2 \text{ Å} = 0.2 \times 10^{-10} \text{ m. } \Delta p = ?$$

We have,
$$\Delta x \, \Delta p \approx \frac{h}{2\pi}$$
 or $\Delta p = \frac{h}{2\pi \Delta x}$

$$\Delta p = \frac{6.626 \times 10^{-34}}{2\pi (0.2 \times 10^{-10})} = 5.274 \times 10^{-24} \text{ kg ms}^{-1}.$$

Example 2. An electron has a speed of 600 ms⁻¹ with an accuracy of 0.005 %. Calculate the certainty with which we can locate the position of the electron. $h = 6.6 \times 10^{-34}$ Js and $m = 9.1 \times 10^{-31}$ kg.

Momentum of the electron = $mv = 9.1 \times 10^{-31} \times 600 \text{ kg ms}^{-1}$.

$$\Delta p = {0.005' \choose 100} mv = (5 \times 10^{-5})(9.1 \times 10^{-31} \times 600) \text{ kg ms}^{-1}$$

From uncertainty principle, $\Delta x \Delta p \approx h/2\pi$

$$\Delta x = \frac{h}{2\pi\Delta p} = \frac{6.6 \times 10^{-34}}{2\pi (5 \times 10^{-5} \times 9.1 \times 10^{-31} \times 600)}$$
$$= 0.003846 \text{ m}.$$

Example 3. The lifetime of an excited state of an atom is about 10⁻⁸ sec. Calculate the minimum uncertainty in the determination of the energy of the excited state.

We have, $\Delta E \Delta t \ge h/2\pi$.

Unit—I WAVE MECHANICS Schoolinges Type constitution of Wave Mechanics equations

7.7. Basic postulates of Wave Mechanics

In the development of Wave Mechanics, there are certain basic postulates, which are of fundamental importance. The fundamental postulates are three in number. Other wave properties follow from them.

(1) Each dynamical variable relating to the motion of a particle can be represented by a linear operator.

Explanation. In classical Physics, certain definite functions of suitable variables are associated with each observable quantity. Thus (x, y, z) are associated with position, mv is associated with momentum, $\frac{1}{2}mv^2$ is associated with K.E. and so on. Similarly, in wave mechanics and quantum mechanics, certain operators are associated with observable quantities. For the x-component of the linear momentum of a particle which has a classical expression $p_x = m \left(\frac{dx}{dt} \right)$ we have a quantum mechanical operator $-i \left(\frac{h}{2\pi} \right) \frac{\partial}{\partial x}$. In the vector form, this operator is $-i\left(\frac{h}{2\pi}\right)\nabla$ For angular momentum we can write the operator as $(\mathbf{r} \times \mathbf{p}) = -i\left(\frac{h}{2\pi}\right)(\mathbf{r} \times \nabla)$. Similarly, for the observable total energy, the classical representation is $\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$ +V(x, y, z) and the quantum mechanical $-\frac{(h/2\pi)^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z).$ An operator tells us what operation to carry out on the quantity that follows it. The operator $i\left(\frac{h}{2\pi}\right)\frac{\partial}{\partial t}$ instructs us to take the partial derivative of what comes after it with respect to t and multiply the result by $i\left(\frac{h}{2\pi}\right)$.

Table 7.1 summarises the quantum operators for several physical quantities.

Table 7.1. Quantum operators

Quantity	Classical definition	Quantum operator
Posițion	sky = siperrati = o mô	r r respective and
Momentum	p p	- i - V
Angular momentum		
Kinetic energy	$p^2/2m$	$-\left(h^2/8\pi^2m\right)\nabla^2$
Total energy	$p^2/2m + E_{I^*}(\mathbf{r})$	$-\left(h^2/8\pi^2m\right)\nabla^2+E_p\left(\mathbf{r}\right)$
re get	wise with seper to a, w	C. Henri mang E

- (2) A linear eigenvalue equation can be always linked with each operator. Example. The total energy operator is $i\left(\frac{h}{2\pi}\right)\frac{\partial}{\partial t}$. Consider the eigen value equation $i\left(\frac{h}{2\pi}\right)\frac{\partial \psi}{\partial t}=E\psi$. Here ψ is said to be an eigenfunction of the operator $i\left(\frac{h}{2\pi}\right)\frac{\partial}{\partial t}$ and E is called the corresponding energy eigenvalue.
- (3) In general, when a measurement of a dynamical quantity a is made on a particle for which the wave function is ψ, we get different values of a during different trials. This is in conformity with the uncertainty principle. The most probable value of a is given by

$$\langle a \rangle = \int_{0} \psi * \hat{A} \psi \ dV$$

- (1)

where \hat{A} is the operator associated with the quantity a and ψ^* is the omptex conjugate of ψ . The quantity $\langle a \rangle$ is called the expectation value of A (that is the value of a obtained in the majority of the trials). The expectation value of momentum and energy may be found by using the corresponding differential operator. Thus

$$\langle \vec{p} \rangle = \int_{-\infty}^{\infty} \psi^* \left(-\frac{ih}{2\pi} \nabla \right) \psi \, dx \, dy \, dz$$

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^* \left(i \frac{h}{2\pi} \frac{\partial}{\partial t} \right) \psi \, dx \, dy \, dz$$

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7.8. Derivation of Time-dependent form of Schrodinger equation

The quantity that characterises the de Broglie waves is called the wave function. It is denoted by Ψ . It may be a complex function. Let us assume that Ψ is specified in the x direction by

$$\Psi = Ae^{-i\alpha(t-x/v)} \qquad \dots (1)$$

If v is the frequency, then $\omega = 2\pi v$ and $v = v\lambda$.

$$\Psi = Ae^{-2\pi i(vr - x/\lambda)} \qquad ...(2)$$

Let E be the total energy and p the momentum of the particle. Then E = hv and $\lambda = h/p$. Making these substitutions in Eq. (2).

$$\Psi = Ae^{-(2\pi i/h)(Et-\mu x)} \qquad ...(3)$$

Eq. (3) is a mathematical description of the wave equivalent of an unrestricted particle of total energy E and momentum p moving in the +x direction.

Differentiating Eq. (3) twice with respect to x, we get

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2 p^2}{h^2} \psi \qquad \dots (4)$$

Differentiating Eq. (3) once with respect to t, we get

$$\frac{\partial \Psi}{\partial t} = -\frac{2\pi i E}{h} \Psi \qquad ...(5)$$

At speeds small compared with that of light, the total energy E of a particle is the sum of its kinetic energy $p^2/2m$ and its potential energy V. V is in general a function of position x and time t.

$$E = \frac{p^2}{2m} + V \qquad ...(6)$$

Multiplying both sides of Eq. (6) by ψ we get

$$E\psi = \frac{p^2\psi}{2m} + V\psi \qquad ...(7)$$

From Eqs. (5) and (4) we see that

$$E\psi = -\frac{h}{2\pi i} \frac{\partial \psi}{\partial t} \qquad ...(8)$$

and

$$p^2 \psi = -\frac{h^2}{4\pi^2} \frac{\partial^2 \psi}{\partial x^2} \qquad ...(9)$$

Substituting these expressions for $E\psi$ and $p^2\psi$ into Eq. (7) we obtain

$$-\frac{h}{2\pi i}\frac{\partial \psi}{\partial t} = -\frac{h^2}{8\pi^2 m}\frac{\partial^2 \psi}{\partial x^2} + V\psi$$

$$\frac{ih}{2\pi} \frac{\partial \Psi}{\partial t} = -\frac{h^2}{8\pi^2 m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \qquad ...(10)$$

Eq. (10) is the time-dependent form of Schrodinger's equation.

In three dimensions the time-dependent form of Schrodinger's equation is

$$\frac{ih}{2\pi} \frac{\partial \Psi}{\partial t} = -\frac{h^2}{8\pi^2 m} \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V \Psi$$

Schrodinger's equation: Steady-state form

In a great many situations the potential energy of a particle does not depend upon time explicitly. The forces that act upon it, and hence V, vary with the position of the particle only. When this is true, Schrodinger's equation may be simplified by removing all reference to t. The one-dimensional wave function ψ of an unrestricted particle may be written in the form

$$\psi = Ae^{-(2\pi i/h)(Et - px)}$$

$$= Ae^{-(2\pi iE/h)t} \cdot e^{+(2\pi ip/h)x}$$

$$\therefore \qquad \psi = \psi_0 e^{-(2\pi iE/h)t} \qquad \dots (1)$$

Here, $\psi_0 = Ae^{+(2\pi i p/h)x}$. That is, Ψ is the product of a position dependent function Ψ_0 and a time-dependent function $e^{-(2\pi i E/h)t}$

Differentiating Eq. (1) with respect to t, we get

$$\frac{\partial \Psi}{\partial t} = -\frac{2\pi i E}{h} \Psi_0 e^{-(2\pi i E/h)t} \qquad ...(2)$$

Differentiating Eq. (1) twice with respect to x, we get

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial^2 \psi_0}{\partial x^2} e^{-(2\pi i E/h)t} \qquad \qquad --(3)$$

We can substitute these values in the time-dependent form of Schrodinger's equation

$$\frac{ih}{2\pi} \frac{\partial \Psi}{\partial t} = -\frac{h^2}{8\pi^2 m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi.$$

$$E\Psi_0 e^{-(2\pi i E/h)t} = -\frac{h^2}{8\pi^2 m} \frac{\partial^2 \Psi_0}{\partial x^2} e^{-(2\pi i E/h)t} + V\Psi_0 e^{-(2\pi i E/h)t}$$

Dividing through by the common exponential factor, we get

$$\frac{\partial^2 \psi_0}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi_0 = 0 \qquad \dots (4)$$

Eq. (5) is the steady-state form of Schrodinger's equation.

In three dimensions it is

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$$\nabla^2 \psi_0 + \frac{8\pi^2 m}{h^2} (E - V) \psi_0 = 0 \qquad ...(5)$$

Usually it is written in the form

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

7.9 Properties of the wave function

Physical significance of Ψ . The probability that a particle will be found at a given place in space at a given instant of time is characterised by the function $\Psi(x,y,z,t)$. It is called the wave function. This function can be either real or complex. The only quantity having a physical meaning is the square of its magnitude $P = |\Psi|^2 = \Psi\Psi$ *where Ψ * is the complex conjugate of Ψ . The quantity P is the probability density. The probability of finding a particle in a volume dx, dy, dz, is $|\Psi|^2 dx dy dz$. Further, since the particle is certainly to be found somewhere in space

$$\iiint |\Psi|^2 dx \cdot dy \cdot dz = 1$$

the triple integral extending over all possible values of x, y, z. A wave function (Ψ) satisfying this relation is called a normalised wave function.

Orthogonal and normalised wave functions. If the product of a function Ψ_1 (x) and the complex conjugate Ψ_2^* (x) of a function Ψ_2 (x) vanishes when integrated with respect to x over the interval $a \le x \le b$ that is, if

$$\int \Psi_2^*(x) \Psi_1(x) dx = 0$$

then $\psi_1(x)$ and $\psi_2(x)$ are said to be orthogonal in the interval (a, b).

We know that the probability of finding a particle in the volume element dV is given by $\Psi \Psi * dV$. The total probability of finding the particle in the entire space is, of course, unity, i.e.,

$$\int |\Psi|^2 dV = 1.$$

where the integration extends over all space. The above equation can also be written as

$$|\Psi\Psi^* dV = 1.$$

Any wave function satisfying the above equation is said to be normalised to unity or simply normalised.

Very often Ψ is not a normalized wave function. We know that it is possible to multiply Ψ by a constant A, to give a new wave function, $A\Psi$, which is also a solution of the wave equation. Now the problem is to choose the proper value of A such that the new wave function is a normalized function. In order that it is a normalized function, it must meet the requirement

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

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

IAlis known as normalizing constant.

To arrive at results consistent with physical observations, several additional requirements are imposed on the wave function $\Psi(x)$:

- 1. It must be well behaved, that is, single-valued and continuous everywhere.
- 2. If $\Psi_1(x)$, ... $\psi_n(x)$ are solutions of Schrodinger equation, then the linear combination $\psi(x) = a_1 \psi_1(x) + a_2 \psi_2(x) + ...a_n \psi_n(x)$ must be a solution.
 - 3. The wave function $\psi(x)$ must approach zero as $x \to \pm \infty$

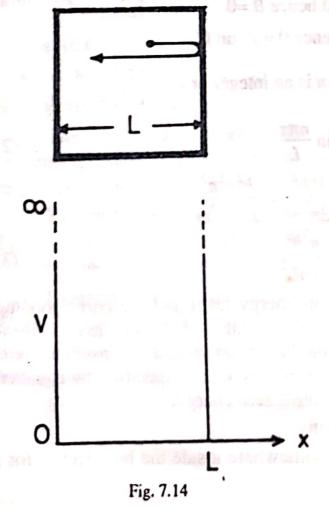
Eigenfunctions and Eigenvalues. Schrodinger's time-independent equation is an example of a type of differential equation called an eigenvalue equation. In general, we can write an eigenvalue equation as

$$F_{op}\Psi = f\Psi$$

The differential operator F_{op} operates on a function ψ , and this yields a constant f times the function. The function ψ is then called an eigenfunction of the operator F_{op} , and the corresponding value for f is called the eigenvalue.

SIMPLE APPLICATIONS OF SCHRODINGER'S EQUATION

7.10. The particle in a box [Infinite Square Well Potential]



Consider a particle moving inside a box along the x-direction. The particle is bouncing back and forth between the walls of the box. The box has insurmountable potential barriers at x = 0 and x = L. i.e., the box is supposed to have walls of infinite height at x = 0 and x = L (Fig. 7.14). The particle has a mass m and its position x at any instant is given by 0 < x < L.

The potential energy V of the particle is infinite on both sides of the box. The potential energy V of the particle can be assumed to be zero between x = 0 and x = L.

In terms of the boundary conditions imposed by the problem, the potential function is

$$V = 0 \text{ for } 0 < x < L$$

$$V = \infty \text{ for } x \le 0$$

$$V = \infty \text{ for } x \ge L$$

The particle cannot exist outside the box and so its wave function Ψ is 0 for $x \le 0$ and $x \ge L$. Our task is to find what Ψ is within the box, viz., between x = 0 and x = L.

Within the box, the Schrodinger's equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0.$$

Putting $\frac{8\pi^2 mE}{h^2} = k^2$, the equation becomes

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0.$$

The general solution of this equation is

$$\Psi = A \sin kx + B \cos kx \qquad \dots (1)$$

The boundary conditions can be used to evaluate the constants A and B in equation (1).

$$\Psi = 0$$
 at $x = 0$ and hence $B = 0$
 $\Psi = 0$ at $x = L$. Hence $0 = A \sin kL$

Since $A \neq 0$, $kL = n\pi$ where n is an integer or $k = \frac{n\pi}{L}$.

Thus
$$\psi_n(x) = A \sin \frac{n\pi x}{L} \qquad ...(2)$$
The energy of the particle
$$E_n = \frac{k^2 h^2}{8\pi^2 m} = \frac{h^2 n^2 \pi^2}{L^2 8\pi^2 m}$$

$$E_n = \frac{n^2 h^2}{8mL^2} \qquad ...(3)$$

For each value of n, there is an energy level and the corresponding wavefunction is given by equation(2). Each value of E_n is called an eigenvalue and the corresponding Ψ_n is called eigenfunction. Thus inside the box, the particle can only have the discrete energy values specified by equation (3). Note also that the particle cannot have zero energy.

The particle in a box: Wave functions

It is certain that the particle is somewhere inside the box. Hence for a normalised wave function

i.e.,
$$\int_{0}^{L} \psi * \psi \ dx = 1 \quad i.e., \quad A^{2} \int_{0}^{L} \sin^{2} \left(\frac{n\pi x}{L}\right) dx = 1$$
or
$$A^{2} \int_{0}^{L} \left(\frac{1 - \cos 2n\pi x/L}{2}\right) dx = 1 \quad \text{or } A^{2} \frac{L}{2} = 1$$
or
$$A = \sqrt{\frac{2}{L}}$$

$$\therefore \text{ The normalised wave functions of the particle } = \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

The normalised wave functions Ψ_1 Ψ_2 and Ψ_3 are plotted in Fig. 7.15.

Example 1. Calculate the permitted energy levels of an electron, in a box I Å wide.

Here, m = mass of the electron $= 9.1 \times 10^{-31} \text{ kg};$

$$L = 1 \text{ Å} = 10^{-10} \text{ m}.$$

$$E_0 = ?$$

.. The permitted electron ener-

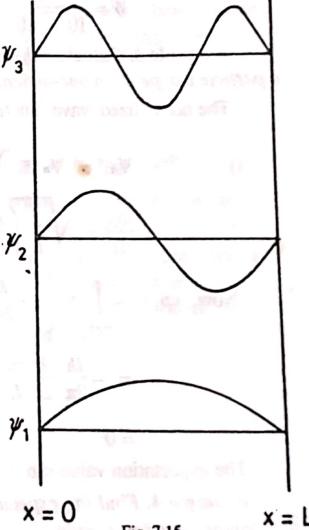
$$gies = E_n = \frac{n^2 h^2}{8mL^2}$$

$$= \frac{n^2 (6.626 \times 10^{-34})^2}{8(9.1 \times 10^{-31}) (10^{-10})^2}$$

$$= 6 \times 10^{-18} \, n^2 \, J = 38 n^2 \, eV.$$

minimum energy, electron can have, is $E_1 = 38 \text{ eV}$, corresponding to n = 1.

The other values of energy are $E_2 = 4E_1 = 152 \text{ eV}, E_3 = 9E_1 = 342$ eV and so on.



x = LFig. 7.15

Example 2. A particle is moving in a one-dimensional box (of infinite height) of width 10 A. Calculate the probability of finding the particle within an interval of 1 A at the centre of the box, when it is in its state of least energy.

The wave function of the particle in the ground state (n = 1) is

of \alpha-decay exhibited by radioactive nuclei.

Example. The potential barrier problem is a good approximation to the problem of an electron trapped inside but near the surface of a metal. Calculate the probability of transmission that a 1.0 eV electron will penetrate a potential barrier of 4.0 eV when the barrier width is 2.0 Å.

From equation (7) the transmission coefficient is

$$T \approx 16 \left(\frac{1.0 \text{ eV}}{4.0 \text{ eV}} \right) \left(1 - \frac{1.0 \text{eV}}{4.0 \text{eV}} \right)$$

$$\times \exp \left[-\frac{2 \times 2 \times 10^{-10} \, m}{1.05 \times 10^{-34} \, Js} \sqrt{2(9.1 \times 10^{-31} \, kg) \, (4-1) \, (1.6 \times 10^{-19} \, J)} \right]$$

$$\approx 0.084$$

Thus, only about eight 1.0 eV electrons, out of every hundred, penetrate the barrier.

7.13. Linear harmonic oscillator

Consider a particle executing simple harmonic motion along the x direction and let k be the restoring force per unit displacement.

The P.E. of the particle =
$$\int_{0}^{x} kx \, dx = \frac{1}{2} kx^{2}$$
.

The Schrodinger equation for the harmonic oscillator is

$$\frac{d^2 \Psi}{dx^2} + \frac{8\pi^2 m}{h^2} \left(E - \frac{1}{2} kx^2 \right) \Psi = 0 \qquad ...(1)$$

It is convenient to simplify Eq. (1) by introducing the dimensionless quantities

$$y = \left(\frac{1}{h/2\pi} \sqrt{km}\right)^{1/2} x = \sqrt{\frac{2\pi mv}{h/2\pi}} x$$
 ...(2)

and

$$\alpha = \frac{2E}{h/2\pi} \sqrt{\frac{m}{k}} = \frac{2E}{h\nu} \qquad \dots (3)$$

where v is the classical frequency of the oscillation given by

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

In terms of y and a, Schrodinger's equation becomes

$$\frac{d^2\psi}{dy^2} + (\alpha - y^2)\psi = 0 \qquad ...(4)$$

To solve this equation, a solution of the form below can be tried:

$$\psi = f(y) e^{-y^2/2}$$
 ...(5)

where f(y) is a function of y that remains to be found.

By inserting the Y of Eq. (5) in Eq. (4) we obtain

$$\frac{d^2f}{dy^2} - 2y \frac{df}{dy} + (\alpha - 1)f = 0. \qquad ...(6)$$

which is the differential equation that f obeys.

Writing $(\alpha - 1) = 2n$, Eq. (6) becomes,

This is a standard mathematical equation known as Hermite's equation. The solutions of Eq. (7) are called Hermite's Polynomials, given by

$$H_n(y) = f(y) = (-1)^n \exp y^2 \frac{d^n}{dy^n} [\exp(-y^2)]$$
 ...(8)

The eigen functions of harmonic oscillator, therefore, are the following:

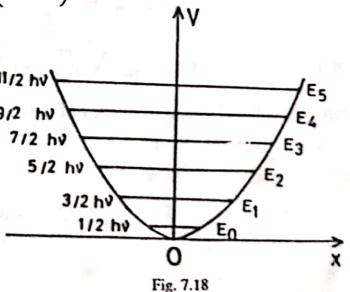
$$\Psi_n(y) = NH_n(y) \exp(-y^2/2)$$
 ...(9)

where N is a normalisation constant.

The eigen values (permitted values of the total energy) are given by.

$$E_n = \left(n + \frac{1}{2}\right)hv, \quad n = 0, 1, 2, 3, \dots (10)$$

The energy of a harmonic oscillator is thus quantised in steps of hv. The energy levels here are even- 9/2 hv ly spaced (Fig. 7.18). We 7/2 hv note that, when n = 0, $E_0 = 5/2 \frac{1}{2} hv$ which is the lowest value of energy the oscillator can have. This value is called the zero point energy.



The Harmonic Oscillator Wave Functions. Each wave function Ψ_n consists of a polynomial $H_n(y)$ (called a Hermite polynomial), the exponential factor $\frac{1}{2}$ and a numerical coefficient which is needed for Ψ_n to meet the normalisation condition

$$\int |\psi_n|^2 dy = 1 \quad n = 0, 1, 2 \quad ...(11)$$

The general formula for the nth wave function is

$$\Psi_n = \left(\frac{2mv}{h/2\pi}\right)^{1/4} (2^n n!)^{-1/2} H_n(y) e^{-y^2/2} \dots (12)$$

The first four Hermite polynomials $H_n(y)$ are listed in table 7.2, and the corresponding wave functions are plotted in Fig. 7.19. The vertical lines show the limits -A and +A between which a classical oscillator with the same energy would vibrate.

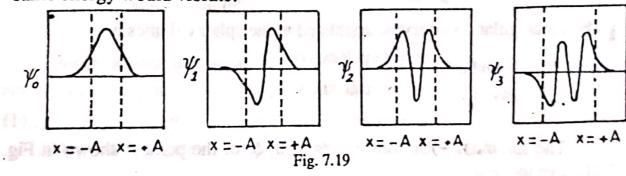


Table 7.2. Some Hermite polynomials

n	H _n (y)	E _n
0	out of the Mark to the	$\frac{1}{2}$ hv
1	2y	$\frac{3}{2}$ hv
2	$4y^2-2$	5 hv
3	$8y^3 - 12y$	$\frac{7}{2}$ hv

7.14. The Hydrogen Atom

The hydrogen atom consists of a proton around which the electron revolves. The proton is assumed at rest at the origin of a rectangular coordinate system, and the electron is orbiting around the fixed proton at a radius r under the influence of the attractive coulomb field of the system. The potential energy function due to the coulomb field is $V(r) = -e^2/4\pi \, \varepsilon_o r$. From the viewpoint of quantum mechanics, the electron is represented by a wave system bounded by the potential well of the coulomb field. This circumstance results in a set of permitted standing wave systems, each corresponding to a particular possible value of the total energy.

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1. Modern Physics, R. Murugesan, 2002, S.Chand & Company Ltd, Ramnagar, New Delhi- 110 055