UNIT 5

PRINCIPLES OF QUANTUM MECHANICS

4.1.1 Wave and particle duality

A particle has mass, it is located at some definite point, it can move from one place to another, it gives energy when slowed down or stopped. Thus, the particle is specified by

(1) Mass m
(2) Velocity v
(3) Momentum p and
(4) Energy E.

A wave is spread out over a relatively large region of space , it cannot be said to be located just here and there, it is hard to think of mass being associated with a wave. Actually a wave is nothing but a rather spread out disturbance. A wave is specified by its

(1) Frequency
(2) Wavelength,
(3) Phase of wave velocity,
(4) Amplitude and
(5) Intensity

Considering the above facts, it appears difficult to accept the conflicting ideas that radiation has a dual nature, i.e., radiation is a wave which is spread out over space and also a particle which is localized at a point in space. However, this acceptance is essential because radiation sometimes behaves as a wave and at other times as a particle as explained below:

(1) Radiations including visible light, infra-red, ultraviolet, X-rays, etc. behave as waves in experiments based on interference, diffraction, etc. This is due to the fact that these phenomena require the presence of two waves at the same position at the same time. Obviously, it is difficult for the two particles to occupy the same position at the same time. Thus, we conclude that radiations behave like wave..

(2) Planck's quantum theory was successful in explaining black body radiation, the photo electric effect, the Compton Effect, etc. and had clearly established that the radiant energy, in its interaction with matter, behaves as though it consists of corpuscles. Here radiation interacts with matter in the form of photon or quanta. Thus, we conclude that radiations behave like particle.

4.1.2 de–Broglie Hypothesis

In the Newton time, matter and radiation both were assumed to consist of particles. With the discovery of phenomena like interference, diffraction and polarization it was established that light is a kind of a wave motion.

In the beginning of 20^{th} century some new phenomena (photoelectric effect, Compton effect, etc.) were discovered which could not be explained on the basis of wave theory. These phenomena were explained on the basis of quantum theory in which light quanta or photons are endowed corpuscular properties – mass ($h\nu/c^2$), velocity v and momentum $h\nu/c$. But, when the photon theory was applied to phenomenon such as interference, diffraction, etc. (which have been fully explained on wave theory) it proved helpless to explain them. Thus, light has a dual nature, i.e., it possesses both particle and wave properties. In some phenomena corpuscular nature predominates while in others wave nature predominates. The manifest of properties depends upon the conditions under which the particular phenomena occur. But wave and particle never expected to appear together.

Louis de- Broglie in 1924 extended the wave particle parallelism of light radiations to all the fundamental entities of Physics such as electrons, protons, neutrons, atoms and molecules etc. He put a bold suggestion that the correspondence between wave and particle should not confine only to electromagnetic radiation, but it should also be valid for material practices, i.e. like radiation, matter also has a dual (i.e., particle like and wave like) character.

In his doctoral thesis de-Broglie wrote that there is an intimate connection between waves and corpuscles not only in the case of radiation but also in the case of matter. A moving particle is always associated with the wave and the particle is controlled by waves. This suggestion was based on the fact that nature loves symmetry, if radiation like light can act like wave some times and like a particle at other times, then the material particles (e.g., electron, neutron, etc.) should act as waves at some other times. These waves associated with particles are named de- Broglie waves or matter waves.

4.1.3 Expression for de- Broglie wavelength

The expression of the wavelength associated with a material particle can be derived on the analogy of radiation as follows:

Considering the plank's theory of radiation, the energy of photon (quantum) is

$$E = h\upsilon = \frac{hc}{\lambda} \qquad \rightarrow (1)$$

Where c is the velocity of light in vacuum and λ is its wave length.

According to Einstein energy – mass relation

$$E = mc^2 \qquad \rightarrow (2)$$

$$\lambda = \frac{h}{mc} = \frac{h}{p} \qquad \rightarrow (3)$$

Where mc = p is momentum associated with photon.

If we consider the case of material particle of mass m and moving with a velocity v , i.e momentum mv, then the wave length associated with this particle (in analogy to wave length associated with photon) is given by

$$\lambda = \frac{h}{mv} = \frac{h}{p} \qquad \rightarrow (4)$$

Different expressions for de-Broglie wavelength

(a) If E is the kinetic energy of the material particle then

$$E = \frac{1}{2}mv^2 = \frac{1}{2}\frac{m^2v^2}{m} = \frac{p^2}{2m}$$

$$\Longrightarrow \quad p^2 = 2mE \text{ or } \quad p = \sqrt{2mE}$$

Therefore de- Broglie wave length $\lambda = \frac{h}{\sqrt{2mE}}$ $\rightarrow (5)$

(b) When a charged particle carrying a charge 'q' is accelerated by potential difference v, then its kinetic energy K .E is given by

$$E = qV$$

Hence the de-Broglie wavelength associated with this particle is

$$\lambda = \frac{h}{\sqrt{2mqV}} \quad \rightarrow (6)$$

For an electron $q = 1.602\times10^{-19}$

Mass $m = 9.1 \text{ X } 10^{-31}$ kg

$$\therefore \quad \lambda = \frac{6.626\times10^{-34}}{\sqrt{2\times9.1\times10^{-31}\times1.602\times10^{-19}V}}$$

$$= \sqrt{\frac{150}{V}} = \frac{12.26}{\sqrt{V}} \text{ A}^0 \quad \rightarrow (7)$$

4.1.4 Properties of Matter Waves

Following are the properties of matter waves:

(a) Lighter is the particle, greater is the wavelength associated with it.

(b) Smaller is the velocity of the particle, greater is the wavelength associated with it.

(c) When v = 0, then $\lambda = \infty$, i.e. wave becomes indeterminate and if v = ∞ then $\lambda = 0$. This shows that matter waves are generated only when material particles are in motion.

(d) Matter waves are produced whether the particles are charged particles or not ($\lambda = \frac{h}{mv}$ is independent of charge). i.e., matter waves are not electromagnetic waves but they are a new kind of waves .

(e) It can be shown that the matter waves can travel faster than light i.e. the velocity of matter waves can be greater than the velocity of light.

(f) No single phenomenon exhibits both particle nature and wave nature simultaneously.

4.1.5 Distinction between matter waves and electromagnetic waves

S.No	Matter Waves	Electromagnetic Waves
1	Matter waves are associated with moving particles (charged or uncharged)	Electromagnetic waves are produced only by accelerated charged particles.
2	Wavelength depends on the mass of the particle and its velocity, $\lambda = \frac{h}{mv}$	Wavelength depends on the energy of photon
3	Matter waves can travel with a velocity greater than the velocity of light.	Travel with velocity of light c= 3×10^8 m/s

4.	Matter wave is not electromagnetic wave.	Electric field and magnetic field oscillate perpendicular to each other.
5.	Matter wave require medium for propagation, i.e, they cannot travel through vacuum.	Electromagnetic waves do not require any medium for propagation, i.e., they can pass through vacuum.

4.2.1 Davisson and Germer's Experiment

The first experimental evidence of matter waves was given by two American physicists, Davisson and Germer in 1927. The experimental arrangement is shown in figure 3.1(a).

The apparatus consists of an electron gun G where the electrons are produced. When the filament of electron gun is heated to dull red electrons are emitted due to thermionic emissions. Now, the electrons are accelerated in the electric field of known potential difference. These electrons are collimated by suitable slits to obtain a fine beam which is then directed to fall on a large single crystal of nickel, known as target T which is rotated about an angle along the direction of the beam is detected by an electron detector (Faraday cylinder) which is connected to a galvanometer. The Faraday cylinder 'c' can move on a circular graduated scale s between 29^0c to 90^0 to receive the scattered electrons.

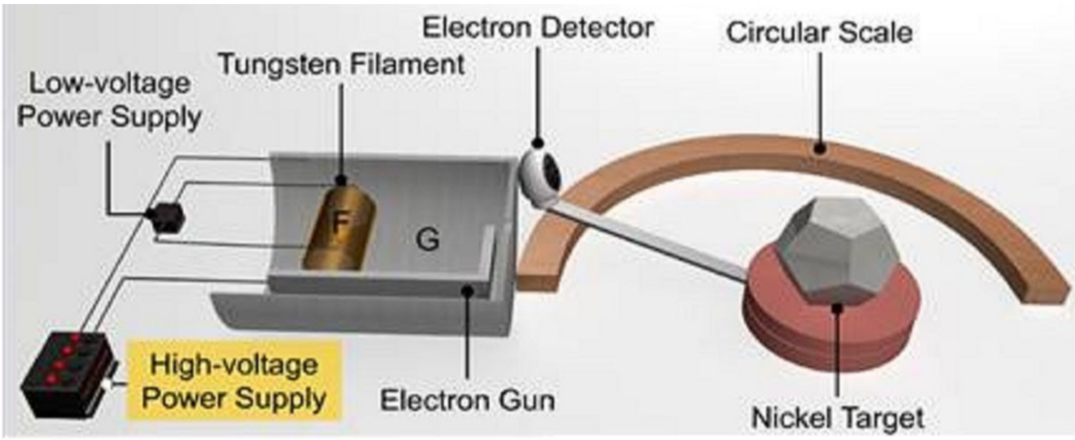

Fig 4.1(a) Davisson and Germer's experimental arrangement for verification of matter waves

First of all, the accelerating potential V is given a low value and the crystal is set at any orbital azimuth (θ). Now the Faraday cylinder is moved to various positions on the scale's' and galvanometer current is measured for each position. A graph is plotted between galvanometer current against angle θ between incident beam and beam entering the cylinder [Figure3.1(b)]. The observations are repeated for different acceleration potentials.

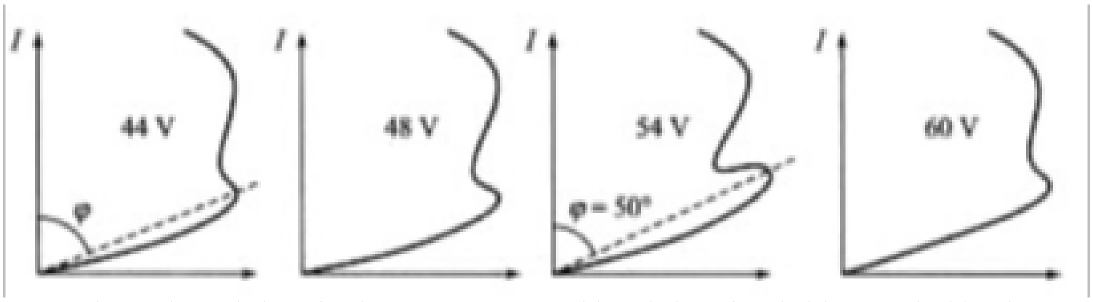

Fig. 4.1(b) Variation of Galvanometer current with variation of angle θ between incident beam and beam entering the cylinder

It is observed that a 'bump' begins to appear in the curve for 44 volts. Following points are observed.

(a) With increasing potential, the bump moves upwards.

(b) The bump becomes most prominent in the curve for 54 volts at $\theta = 50^0$.

(c) At higher potentials, the bumps gradually disappear.

The bump in its most prominent state verifies the existence of electron waves. According to de- Broglie, the wavelength associated with electron accelerated through a potential V is given by

$$\lambda = \frac{12.26}{\sqrt{V}} \quad A^0.$$

Hence, the wavelength associated with an electron accelerated through 54 volt is

$$\lambda = \frac{12.26}{\sqrt{54}} = 1.67\ A^0$$

From X-ray analysis, it is known that a nickel crystal acts as a plane diffraction grating with space $d = 0.91\ A^0$ [see Figure 3.1(c)]. According to experiment, we have diffracted electron beam at $\theta = 50^0$. The corresponding angle of incidence relative to the family of Bragg plane

$$\theta^1 = \frac{180-50}{54} = 65^0$$

Using Bragg's equation (taking n=1), we have

$$\lambda = 2d\sin\theta$$
$$= 2(0.91A^0)\sin 65^0$$

This is in good agreement with the wavelength computed from de-Broglie hypothesis.

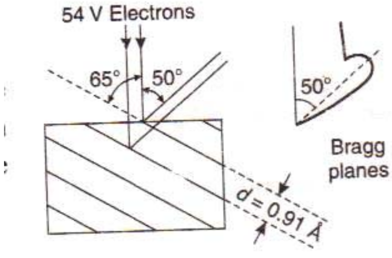

Fig. 4.1(c) Bragg planes in Nickel crystal

As the two values are in good agreement, hence, confirms the de-Broglie concept of matter waves.

4.2.2 G .P. Thomson′s Experiment

The experimental arrangement is as shown in Figure 3.2. High energy electron beam produced by the cathode ‘C’ is accelerated with a potential up to 50kV. A fine pencil of accelerated beam is obtained by allowing it to pass through a narrow slit S and is made to fall on a very thin metallic film F of gold (or silver or aluminum). The electron beam is scattered in different directions by the metallic film and incident on photographic plate P. The entire apparatus is exhausted to a high vacuum so that the electrons may not lose their energy in collision with the molecules of air.

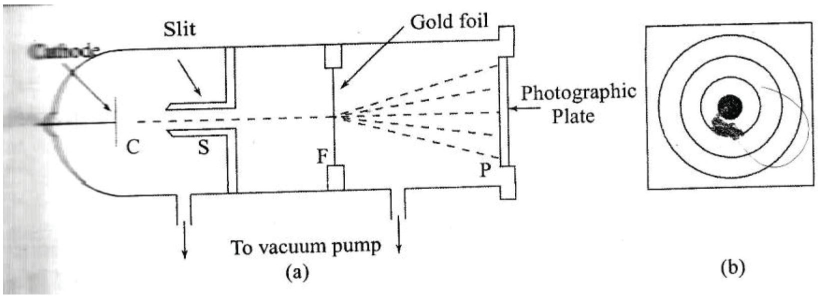

Fig 4.2: (a) G.P.Thomson’s Apparatus, (b) pattern recorded on the photographic plate

Since ordinary metals like gold are micro crystalline in structure, the diffraction pattern produced by them are similar in appearance to the X- ray diffraction powered pattern and consist of a series of well-defined concentric rings about a central spot as shown in figure 4.2(b).

To make sure that this pattern is due to electrons and not due to any possible X - rays generated, the cathode rays in the discharge tube are deflected by magnetic field. It was observed that the diffraction pattern observed on the fluorescent screen placed instead of photographic plate also shifted. This confirmed that the pattern is due to the electrons.

Thomson calculated the wavelength of the de-Broglie waves associated with the cathode rays using the equation

$$\lambda = \frac{12.26}{\sqrt{V}} \text{ A}^0$$

and determined the spacing between the planes in the foils using Bragg’s equation. The results obtained are in good agreement with those from X-ray studies.

4.3 Heisenberg′s Uncertainty Principle

As a direct consequence of the dual nature of matter, in 1927, Heisenberg proposed a very interesting principle known as uncertainty principle.

If a particle is moving, based on classical mechanics, at any instant we can find its momentum at any position. In wave mechanics, a moving particle can be regarded as a wave group. The particle that corresponds to this wave group may be located anywhere within the group at any given time.

In the middle of the group, the probability of finding the particle is more but the probability of finding the particle at any other point inside the wave group is not zero. Narrower the wave group higher will be the accuracy of locating the particle. At the same time, one cannot define the wavelength λ of the wave accurately when the wave group is narrower. Since ($\lambda = \frac{h}{mv}$), measurement of particles momentum (mv = $\frac{h}{\lambda}$) also becomes less accurate.

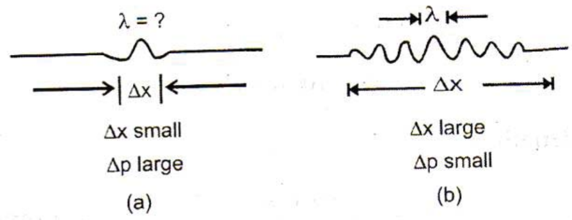

Fig 4.3 (a) A narrow de – Broglie wave group. Since the position can be precisely determined, Δ x is small. As the measurement of is less accurate, Δ p is large. (b) A wide de –Broglie wave group. Measurement of λ is accurate and hence Δ p is small whereas, since wave group is wide, Δ x is large

On the other hand, when we consider a wide wave group, wavelength λ can be well defined hence measurement of momentum becomes more accurate. At the same time, since the width of the wave group is large, locating the position of the particle becomes less accurate.

Thus the uncertainty principle can be stated as ***"it is impossible to know both exact position and exact momentum of an object at the same time".***

If Δx and Δp are the uncertainties in the position and momentum respectively when they are simultaneously measured, then

$$\Delta x \, \Delta p \geq \frac{h}{4\pi}$$

Another form of the uncertainty concerns energy and time. In an atomic process let energy 'E' be emitted during the time interval Δt, If the energy is emitted in the form of electromagnetic waves, we cannot measure frequency υ of the waves accurately in the limited time available . Let the minimum uncertainty in the number of waves that we count in a wave group be one wave.

$$\text{Since frequency} = \frac{number\ of\ waves}{time\ interval}$$

$$\Delta \upsilon = \frac{1}{\Delta t}$$

Hence the corresponding uncertainty in energy

$$\Delta E = h \, \Delta \upsilon$$

$$\Delta E \geq \frac{h}{\Delta t} \quad \text{or} \quad \Delta E \, \Delta t \geq h$$

A more precise calculation based on the nature of wave of wave groups modifies this result to

$$\Delta E \, \Delta t \geq \frac{h}{4\pi}$$

This gives uncertainty in the measurement of energy and time of a process.

Thus the more generalized statement of Heisenberg's uncertainty principle is

“***It is impossible to specify precisely and simultaneously the values of both members of particular pair of physical variables that describe the behavior of an atomic system***”.

4.4.1 Schrodinger's time independent wave equation

Schrodinger developed a differential equation whose solutions yield the possible wave functions that can be associated with a particle in a given situation. This equation is popularly known as Schrodinger equation. The equation tells us how the wave function changes as a result of forces acting on the particle. One of its forms can be derived by simply incorporating the de-Broglie wavelength expression into the classical wave equation.

If a particle of mass ‘m’ moving with velocity v is associated with a group of waves, let ψ be the wave function of the particle. Also let us consider a simple form of progressing wave represented by the equation

$$\psi = \psi_0 \sin(\omega t - kx) \qquad \rightarrow (1)$$

Where $\psi = \psi(x, t)$

ψ_0 is amplitude

Differentiating eq (1) partially with respect to ‘x’, we get

$$\frac{\partial \psi}{\partial x} = -K\, \psi_0 \cos(\omega t - kx)$$

Again differentiating equation (1) with respect to ‘x’

$$\frac{\partial^2 \psi}{\partial x^2} = -K^2\, \psi_0 \sin(\omega t - kx)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi$$

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

Since $k = \frac{2\pi}{\lambda}$, $\quad \frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{\lambda^2} \psi = 0 \qquad \rightarrow (3)$

Eq (2) or Eq (3) is the differential form of the classical wave equation. Now, incorporating de- Broglie wavelength expression $\lambda = \frac{h}{mv}$ in to eq (3), we get

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \qquad \rightarrow (4)$$

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

i.e., $E = K + V$

But $K = \frac{1}{2} mv^2$

$\therefore \quad E = \frac{1}{2} mv^2 + V$

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

$$m^2 v^2 = 2m(E - V) \qquad \rightarrow (5)$$

Substituting eq (5) in eq (4), we get

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m(E - V)}{h^2} \psi = 0 \qquad \rightarrow (6)$$

In quantum mechanics, the value $\frac{h}{2\pi}$ occurs most frequently. Hence we denote $\hbar = \frac{h}{2\pi}$ using this notation, we have

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m(E - V)}{\hbar^2}\psi = 0 \qquad \rightarrow (7)$$

For simplicity, we have considered only one dimensional wave extending eq(7) for a 3 – dimensional wave

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m(E - V)}{\hbar^2}\psi = 0 \qquad \rightarrow (8)$$

Where ψ (x, y, z); here, we have considered only stationary states of ψ after separating the time dependence of ψ

The Laplacian operator is defined as

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad \rightarrow (9)$$

Hence eq (10) can be written as

$$\nabla^2\psi + \frac{2m(E - V)}{\hbar^2}\psi = 0 \qquad \rightarrow (10)$$

This is Schrodinger wave equation. Since time factor doesn't appear, eq(8) or eq(10) is called 'time independent Schrodinger wave equation' in three dimensions.

4.4.2 Physical significance of wave function ψ

(1) The wave function ψhas no direct physical meaning. It is a complex quantity representing the variation of matter wave.

(2) It connects the practical nature and its associated wave nature statically.

(3) $|\psi|^2$ (or $\psi\psi^*$ if function is complex) at a point is proportional to the probability of finding the particle at that point at any given time. The probability density at any point is represented by $|\psi|^2$.

(4) If the particle is present in a volume dxdydz, then $|\psi|^2$ dxdydz =1

If a particle is present somewhere in space

$$\int_{-\infty}^{\infty} \psi^2 \, dx\, dy\, dz = 1$$

$$\text{Or} \qquad \int_{-\infty}^{\infty} \psi\psi * \, dx\, dy\, dz = 1$$

The wave function satisfying the above condition is said to be normalized.

4.5.1 Particle in Infinite square potential well

A free electron trapped in a metal or charge carriers trapped by barriers trapped by the potential barriers of a double hetero junction can be approximated by an electron in an infinitely deep one- dimensional potential well.

Consider one – dimensional potential well of width L as shown in fig. Let the potential

V = 0 inside well and V = ∞ outside the well.

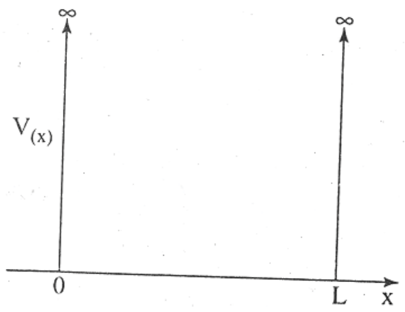

Fig.4.4 Square potential well infinite height

The time independent Schrödinger wave equation in one dimensional case

$$\frac{d^2\psi}{dx^2} + \frac{2m(E - V)}{\hbar}\psi = 0 \qquad \rightarrow (1)$$

For a particle present inside the well where V=0 and $\psi = \psi(x)$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad \rightarrow (2)$$

Let the general solution of eq (2) be

$$\psi(x) = A \sin kx + B \sin kx \qquad \rightarrow (3)$$

Where A and B are constants which can be determined from boundary conditions

$$\left.\begin{array}{ll} & \psi(x) = 0 \text{ at } x = 0 \\ \text{And} & \psi(x) = 0 \text{ at } x = L \\ \text{Since} & \psi(x) = 0 \text{ at } x = 0 \end{array}\right\} \qquad \rightarrow (4)$$

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

$$\Longrightarrow \quad B = 0 \qquad \rightarrow (5)$$

Since $\psi(x) = 0$ at $x = L$

$$0 = A \sin kL$$

Which means A =0 or $\sin kL = 0$ since both A and B cannot be zero, A≠ 0. If A = 0, then $\psi = 0$ everywhere. This means that the particle is not in the well. The only meaningful way to satisfy the condition is

$$\sin kL = 0,$$

or $kL = n\pi$; $n = 1,2,3,\ldots$

$$\therefore \quad k = \frac{n\pi}{L} \qquad \rightarrow (6)$$

Thus, eq (3) simplifies to

$$\psi(x) = A \sin\frac{n\pi}{L}x \qquad \rightarrow (7)$$

Differentiating ψ in eq (7)

$$\frac{d\psi}{dx} = A\frac{n\pi}{L}\cos\frac{n\pi}{L}x$$

Again Differentiating, we get

$$\frac{d^2\psi}{dx^2} = -A\frac{n^2\pi^2}{L^2}\sin\frac{n\pi}{L}x$$

$$\frac{d^2\psi}{dx^2} \quad = \quad -\frac{n^2\pi^2}{L^2}\ \psi \quad = \ 0$$

$$\frac{d^2\psi}{dx^2} \ + \ \frac{n^2\pi^2}{L^2}\ \psi \quad = 0 \qquad \rightarrow (8)$$

Comparing eq (2) and eq (8), we get

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

$$E \ = \ \frac{n^2\ \pi^2\ \hbar^2}{2mL^2}$$

n is called the quantum number. Thus we obtain an important result. The particle cannot possess any value of energy as assumed in classical case, but it possesses only discrete set of energy values.

The energy of the n^{th} quantum level,

$$E_n = \ \frac{n^2\ \pi^2\ \hbar^2}{2mL^2} \ = \ \frac{n^2\ h^2}{8mL^2} \qquad (\text{since } \hbar \ = \ \frac{h}{2\pi}\ ) \qquad \rightarrow (9)$$

The wave functions and the corresponding energy levels of the particles are as suggested in Figure 3.5

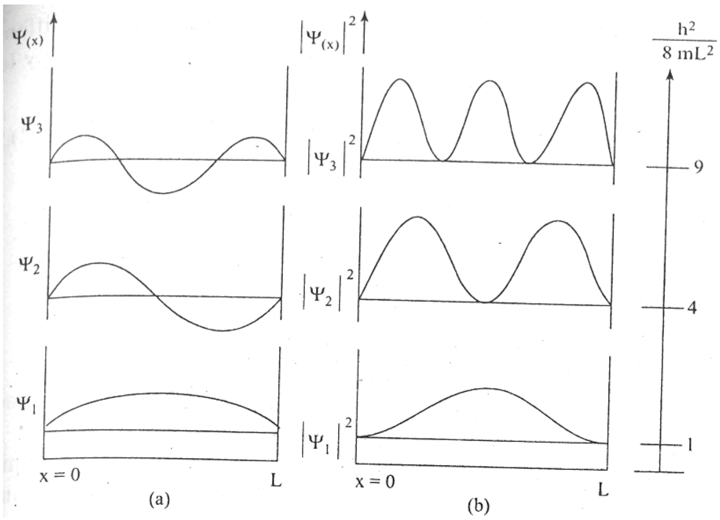

Fig.4.5 Ground state and first two excited states of an electron in a potential well: a) the electron wave functions and b) the corresponding probability density functions. The energies of these three states are shown on the right.

We are still left with an arbitrary constant 'A' in eq (7). It can be obtained by applying normalization condition i.e.; the probability of finding the particle inside the box is unity.

$$\int_0^L |\psi\, x|^2\ dx \quad = \quad 1$$

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

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

$$\frac{A^2}{2}\left[x - \frac{L}{2\pi n} \quad sin\frac{2\pi n x}{L}\right]^L_0 \quad = 1$$

$$\Rightarrow \qquad \frac{A^2}{2}[(L-0) - (0-0)] = 1$$

$$\frac{A^2 L}{2} = 1 \text{ or } A = \sqrt{\frac{2}{L}} \qquad \rightarrow 10)$$

∴ The normalized wave function is

$$\psi_n = \sqrt{\frac{2}{L}}\ \sin\frac{n\pi x}{L} \qquad \rightarrow (11)$$

4.5.2 Particle in Three dimensional potential box

Let us consider the case of a single particle, i.e., a gas molecule of mass m, confined within a rectangular box with edges parallel to X, Y and Z axes as shown in figure.

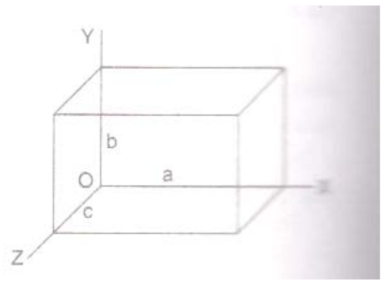

Fig 4.6 Three dimensional potential box

Let the sides of the rectangular box be a, b and c respectively. The particle can move freely within the region $0 < x < a$, $0 < y < b$ and $0 < z < c$, i.e., inside the box where potential V is zero, i.e.,

$V(x, y, z) = 0$, for $0 < x < a$
$V(x, y, z) = 0$, for $0 < y < b$
and $V(x, y, z) = 0$, for $0 < z < c$

The potential rises suddenly to have a large value at the boundaries, i.e., the potential outside the box is infinite.

The Schrodinger wave equation inside the box is given by

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}E\psi = 0 \qquad \rightarrow (1)$$

This is partial differential equation in three independent variables and may be solved by the method of separation of variables. The solution of equation (1) is of the form

$$\psi(x, y, z) = X(x)\, Y(y)\, Z(z) \qquad \rightarrow (2)$$

Where X (x) is a function of x alone, Y(y) is a function of y alone and Z (z) is a function of z alone.

Differentiating ψ in eq (2) partially with respect to 'x', we get

$$\frac{\partial\psi}{\partial x} = \frac{\partial X(x)}{\partial x} \text{Y(y) Z (z)} \qquad \rightarrow (3)$$

Again differentiating eq (3) partially with respect to 'x', we get

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2 X(x)}{\partial x^2} \text{ Y(y) Z (z)}$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2 X(x)}{\partial x^2} \frac{\text{X (x) Y(y) Z (z)}}{X(x)}$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{X}\frac{\partial^2 X}{\partial x^2}\psi \qquad \rightarrow (4)$$

Where X = X(x) and $\psi = \psi$ (x, y, z)

Similarly, $$\frac{\partial^2\psi}{\partial y^2} = \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}\psi \qquad \rightarrow (5)$$

And $$\frac{\partial^2\psi}{\partial z^2} = \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\psi \qquad \rightarrow (6)$$

Substituting eqs.(4),(5) and (6) in eq (1), we get

$$\left[\frac{1}{X}\frac{\partial^2 X}{\partial x^2}\psi + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}\psi + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\psi\right] + \frac{2m}{\hbar^2}\text{E}\psi = 0$$

$$\left[\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right] + \frac{2m}{\hbar^2}\text{E} = 0 \qquad \rightarrow (7)$$

This equation can be written as

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} - \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} \qquad \rightarrow (8)$$

The left hand side of eq (8) is a function of x alone, while the right hand side is a function of y and z and is independent of x. both sides are equal to each other. Both sides are equal to each other. This is possible only when they are separately equal to a constant quantity, i.e.

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = k_x \qquad \rightarrow (9)$$

And $$-\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} - \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} = k_x$$

Or $$\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = -\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} - k_x \qquad \rightarrow (10)$$

In eq (10), the left hand side is a function of y alone while right hand side is a function of z and is independent of y. If the above equation is to be satisfied, both sides must be equal to a constant sayk_y, i.e.

$$\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = k_y \qquad \rightarrow (11)$$

and $$-\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} - k_x = k_y$$

Or $$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = -\frac{2mE}{\hbar^2} - k_x - k_y \qquad \rightarrow (12)$$

Again, we have $$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = k_z \qquad \rightarrow (13)$$

And $$-\frac{2mE}{\hbar^2} - k_x - k_y = k_z$$

Or $$\frac{2mE}{\hbar^2} = -k_x - k_y - k_z \qquad \rightarrow (14)$$

For convenience, introduce

$$k_x = -\frac{2mE_x}{\hbar^2} \quad , \quad k_y =-\frac{2mE_y}{\hbar^2} \quad \text{and} \quad k_z = -\frac{2mz}{\hbar^2}$$

Now, the differential equations in x, y and z coordinates may be written as

$$\frac{\partial^2 X}{\partial x^2} + \frac{2mE_x}{\hbar^2} X = 0 \qquad \rightarrow (15a)$$

$$\frac{\partial^2 Y}{\partial y^2} + \frac{2mE_y}{\hbar^2} Y = 0 \qquad \rightarrow (15b)$$

And $$\frac{\partial^2 Z}{\partial z^2} + \frac{2mE_z}{\hbar^2} Z = 0 \qquad \rightarrow (15c)$$

The general solution of eq [(15a)] will be a sine function of the arbitrary amplitude, frequency and phase, i.e.,

$$X(x) = A \sin (Bx + C) \qquad \rightarrow (16)$$

Where A, B and C are constants whose values are determined by boundary conditions.

$|\psi|^2$ represents the probability of finding the particle at any point within the box. Therefore, $|X(x)|^2$ which is a function of x coordinates only represents the probability of Finding the particle at any point along the X-axis. As the potential is very high at the walls of the box, the probability of finding the particle at the walls will be zero, i.e.,

$$|X(x)|^2 = 0 \text{ when } x = 0 \text{ and } x= a$$

$$X(x) = 0 \text{ when } x = 0 \text{ and } x= a$$

Using the above boundary conditions in eq (16), we have

$$0 = A \sin (0 + C); \quad A \neq 0$$

$\therefore$ Sin C = 0 and $\quad 0 = A\, sin\, (Ba + C)$

\ Or $\quad 0 = \sin Ba . \cos C + \cos Ba . \sin C$

$\quad 0 = \sin Ba \cos C$

$\therefore$ Sin Ba = 0 [since $\sin C = 0$, $\cos C$ is not zero]

$$\leftrightarrow \qquad Ba = n_x\pi$$

$$\text{Or} \quad B = \frac{n_x\pi}{a} \qquad \rightarrow (17)$$

$$\therefore \quad X(x) = A \text{ Sin } \frac{n_x\pi}{a} x \qquad \rightarrow (18)$$

Applying the normalization condition between x=0 to x=a, we have

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

$$\int_0^a \left|A \text{ Sin } \frac{n_x\pi}{a} x\right|^2 dx = 1$$

$$A^2 \int_0^a \text{Sin}^2 \frac{n_x\pi}{a} x \, dx = 1$$

$$\frac{A^2}{2} \int_0^a \left[1 - Cos\, \frac{2\, n_x\pi}{a} x\right] dx = 1$$

$$\frac{A^2}{2} \left[x - \frac{\text{Sin}\frac{2\, n_x\pi}{a}}{\frac{2\, n_x\pi}{a}} \right]_0^a = 1$$

$$\frac{A^2}{2} [a - 0] = 1$$

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

$$\text{Therefore, } X(x) = \sqrt{\frac{2}{a}} \text{ Sin } \frac{n_x\pi x}{a} \qquad \rightarrow (19)$$

Similarly, we can solve equations [15(b)] and [15(c)] to obtain

$$Y(y) = \sqrt{\frac{2}{b}} \text{ Sin } \frac{n_y \pi y}{b} \quad \rightarrow (20)$$

$$Z(z) = \sqrt{\frac{2}{c}} \text{ Sin } \frac{n_z \pi z}{c} \quad \rightarrow (21)$$

The complete wave function ψ_{n_x}, n_y, n_z has the form

$$\psi_{n_x}, n_y, n_z = \sqrt{\frac{2}{a}} \text{ Sin } \frac{n_x \pi}{a} \text{ x } \sqrt{\frac{2}{b}} \text{ Sin } \frac{n_y \pi}{b} \text{ Y } \sqrt{\frac{2}{c}} \text{ Sin } \frac{n_z \pi}{c} \text{ Z}$$

$$= \frac{2\sqrt{2}}{\sqrt{abc}} \text{ Sin } \frac{n_x \pi}{a} \text{ x } \sqrt{\frac{2}{b}} \text{ Sin } \frac{n_y \pi}{b} \text{ Y } \sqrt{\frac{2}{c}} \text{ Sin } \frac{n_z \pi}{c} \text{ Z} \quad \rightarrow (22)$$

The wave function of a particle in a finite box and its probability density are shown in Figure 3.7.

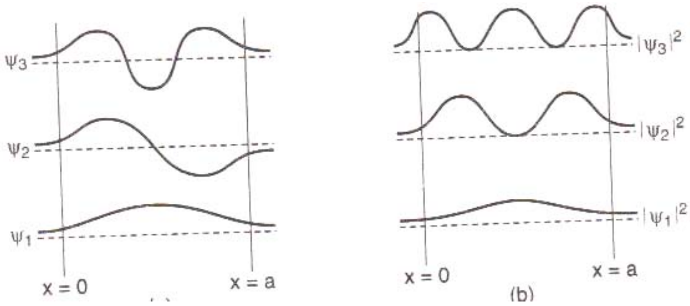

Fig 4.7 a) wave functions and b) probability densities of a particle in three dimensional box

Differentiating eq (19) twice with respect to 'x', we get

$$\frac{\partial^2 X}{\partial x^2} = -[\frac{\pi n_x}{a}]^2 \sqrt{\frac{2}{a}} \text{ Sin } \frac{n_x \pi x}{a} = -[\frac{\pi n_x}{a}]^2 \text{ X(x)} \quad \rightarrow (23)$$

Substituting eq (23) in eq [15(a)], we get

$$-[\frac{\pi n_x}{a}]^2 \text{ X(x)} + \frac{2mE_x}{\hbar^2} \text{ X (x)} = 0$$

$$\text{Or} \quad \frac{2mE_x}{\hbar^2} = [\frac{\pi n_x}{a}]^2$$

$$\text{Or} \quad E_x = \frac{\pi^2 {n_x}^2}{a^2} \frac{h^2}{4\pi^2} \frac{1}{2m}$$

$$E_x = \frac{h^2 {n_x}^2}{8ma^2} \quad \rightarrow (24)$$

$$\text{Similarly,} \quad E_y = \frac{h^2 {n_y}^2}{8mb^2} \quad \rightarrow (25)$$

$$\text{And} \quad E_z = \frac{h^2 {n_z}^2}{8mc^2} \quad \rightarrow (26)$$

The allowed values of total energy are given by

$$E = E_x + E_y + E_z$$

$$= \frac{h^2}{8m^2} [\frac{{n_x}^2}{a^2} + \frac{{n_y}^2}{b^2} + \frac{{n_z}^2}{c^2}] \quad \rightarrow (27)$$

Wheren_x, n_y and n_z denote any set of three positive numbers.

When the box is a cube, i.e., a = b= c, the energy expression is given by

$$E = \frac{h^2}{8ma^2}\left[\frac{{n_x}^2+{n_y}^2+{n_z}^2}{a^2}\right] \rightarrow (28)$$

With n_x, n_y, n_z =

Objective Questions

I choose the correct answer

1. Davisson and germens experiment relates to: [ ]

   (a) Interference (b) Polarization

   (c) Phosphorescence (d) electron diffraction

2. Uncertainty principle was discovered by ___________ [ ]

   (a) Bohr (b) de-Broglie (c) Heisenberg (d) Schrodinger

3. The wavelength if de-Broglie wave associated with an electron accelerated through 50 volts is [ ]

   (a)1 A^0 (b) 1.5 A^0 (c) 1.27 A^0 (d) 1.28 A^0

4. Among the following practices moving with velocity, the particle having shortest wave associated with it is: [ ]

   a) Proton (b) Neutron (c) α-particle (d) $\beta -$ Particle

5. The wavelength associated with a particle moving with velocity v is: [ ]

   (a) λ =h/mv (b)λ =h^2/mv

   (c) λ =mv/h (d) $\lambda = \frac{(mv)^2}{h}$

6.the quantized energy do a particular of mass 'm' confined in one dimensional box of length L is ___________ [ ]

   (a) $\frac{n^2h^2}{8mL^2}$ (b) $\frac{n^2h^2}{8m^2L^2}$

   (c) $\frac{n^2h}{8mL}$ (d) $\frac{n^2h^2}{8Lm^2}$

7 Fermi energy is the of the state at which the probability of electron is____________ at any temperature above ok [ ]

   (a) 1 (b) 0

   (c) 0.5 (d) Any value between 0 and 1

9. If E is the kinetic energy of the material particle of mass ' m' then the de-Broglie wavelength is given by ______________ [ ]

   (a)$\frac{h}{\sqrt{2ME}}$ (b) $\frac{\sqrt{2ME}}{h}$

   (c) $h\sqrt{2ME}$ (d) $\frac{h}{2ME}$

10. If E is the kinetic energy of the material particle of mass 'm' then de-broglie wavelength is given by

[ ]

(a) Lesser than velocity of light (b) Equal to velocity of light
(c) Greater than velocity of light (d) none of these

11. Existence of matter waves was experimentally first demonstrated by [ ]
(a) Newton (b) Planck
(c) de-Broglie (d) Davisson and Germer

12. Wave nature and particle nature called dual nature is exhibited by [ ]
(a)Waves only (b) Particles only
(c)Photons (d) By both particles and waves

16. The lowest energy state of a particle of mass M confined in a linear box of size L is: [ ]
(a) $\frac{h^2}{8mL^2}$ (b) $\frac{2h^2}{8mL^2}$ (c) $\frac{4h^2}{8mL^2}$ (d) $\frac{9h^2}{8mL^2}$

19. The wavelength associated with an electron which has been accelerated from rest application of potential of 900V is [ ]
(a) 0. 613A^0 (b) 0. 365A^0
(c) 0. 4086A^0 (d) None of these

20. The normalized wave function of a particle n a one dimensional potential well is: [ ]
(a) $\sqrt{\frac{L}{2}}\sin\frac{n\pi x}{L}$ (b) $\frac{\sqrt{2}}{L}\sin\frac{n\pi x}{L}$
(c) $\frac{2}{\sqrt{L}}\sin\frac{n\pi x}{L}$ (d) $\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}$

21. When the potential barrier strength is zero, then E-k curve is: [ ]
(a) Continuous parabola
(b) Discrete energy levels
(c) Parabola with discontinuities
(d) Exponentially decaying function of k

II. Fill in the blanks:

1. Uncertainty principle was proposed by _________
2. Lighter the particle, _________the de-Broglie wavelength associated with it.
3. According to uncertainty principle, it is not possible to measure both energy and __________ of a process very accurately and simultaneously.
4. __________ can travel faster than velocity of light.
5. According to Planck's quantum theory, energy is emitted in the form of packets or quanta called ____________
6. One dimensional time independent Schrodinger wave equation is __________

7. The wavelength associated with an electron moving under a potential of 1600V is ________
8. Fermi energy is the energy of the state at which the probability of electron occupation is ________ at any temperature above 0K.
9. At 0K, all the energy levels above Fermi level are ______________
10. Lighter is the particle, ________ is the wavelength associated with it.
11. Three dimensional time independent Schrodinger's wave equation is __________
12. Matter wave is associated with _____________ particle.
13. Wave functions representing ________ are ant symmetric.
14. He^4 atoms obey ___________ statistics.
15. _____________ is the velocity of the particle greater is the wavelength associated with it
16. The subject which deals with the relationship between the overall behavior of the system and the properties of the particles is called __________
17. Single crystal target of nickel is used in ___________ experiment to prove wave nature of electrons.
18. If E_{F_0} is the Fermi-energy of an electron at 0K, then its Fermi – energy at any temperature above 0K is ________________
19. .
20. All the energy levels below Fermi-level are completely filled at a temperature ______
21. Thin metallic film of gold or silver or aluminium is used as target in __________ experiment to prove wave nature of electrons.
22. When an electron moves in a periodic potential of lattice, its mass varies and this mass is called __________of the electron.
23. __________ Model proposed a simpler potential in the form of an array of square wells.
24. The representation of permissible values of K of the electrons in one, two or three dimensions is known as _________________
25. The periodicity of the potential of zone theory of solids is given by __________ theorem.
26. __________ have relatively wide forbidden gaps.
27. __________ have relatively narrow band gaps.
28. According to zone theory of solids, free electrons move inside __________ potential field
29. When the band gap is in the order of 1ev in a solid, it behaves as a ____________
30. __________ have either partially filled valence band or overlap of completely filled valence band with partially filled conduction band.

31. When the band gap is in the order of 7ev in a solid, it behaves as a ___________

Problems

1. **A body at 1500K emits maximum energy at a wavelength 20,000 A^0.If the sun emits maximum temperature of wavelength 5500 A^0, what would be the temperature of the Sun.**

   Solution: According to Wien's displacement law,

   $\lambda_m T$=constant

   Or $\lambda_m T = \lambda_m^1 T^1$

   $T^1 = \frac{\lambda_m T}{\lambda_m^1} = \frac{20000 \text{ X } 1500}{5500}$ =5454K

2. **At what temperature we can expect a 10% probability that electrons in silver have an energy which is 1% above the Fermi energy? (The Fermi energy of silver is 5.5eV.)**

   Solution: probability function

   $$F(E) = \frac{1}{1+exp\left(\frac{E-E_F}{K_T}\right)}$$

   Given data: F (E) =10%=0.1

   $E_F = 5.5\text{eV}$

   $E = E_F + \frac{1}{100} E_F$

   $(5.5+0.055) = 5.555\text{eV}$

   $E - E_F = 0.055\text{eV} = 0.055\times1.6\times10^{-19}\text{J}$

   Substituting in the formula

   $$0.1 = \frac{1}{1+exp\left(\frac{0.055\times1.6\times10^{-19}}{T\times1.38\times10^{-23}}\right)}$$

   i.e. $$0.1 = \frac{1}{exp\left(\frac{637.7}{T}\right)+1}$$

   $$exp\left(\frac{637.7}{T}\right)+1 = 10$$

   $$\left(\frac{637.7}{T}\right) = \ln 9$$

   $$T = \frac{637.7}{T} = \ln 9$$

   $$T = \frac{637.7}{\ln 9}$$

   $$T = \frac{637.7}{2.197} = 290.2\text{K}$$

3. **Evaluate the Fermi function for an energy KT above the Fermi energy.**

Solution: Fermi function F (E) = $\frac{1}{1+exp\left(\frac{E-E_F}{K_T}\right)}$

Given that E-E_F =KT

$$F(E) = \frac{1}{1+exp(1)} = \frac{1}{1+2.718}$$

$$= \frac{1}{3.718}$$

$$= 0.269$$

4. **Calculate the wavelength of an electron raised to a potential 1600V.**

Solution: de-Broglie wavelength

$$\lambda = \frac{12.26}{\sqrt{v}} A^0$$

$$= \frac{12.26}{\sqrt{1600}}$$

$$= \frac{12.26}{40}$$

$$= 0.3065A^0$$

5. **If the kinetic energy of the neutron is 0.025eV calculate its de-Broglie wavelength (mass of neutron =1.674X10^{-27} Kg)**

Solution: Kinetic energy of neutron

$$E = \frac{1}{2} mv^2 = 0.025eV$$

$$= 0.025 \times 1.6x10^{-19} J$$

$$v = \left(\frac{2X0.025 \times 1.6 \times 10^{-19}}{1.674 \times 10^{-27}}\right)^{\frac{1}{2}} = (0.04779 \times 10^8)^{\frac{1}{2}}$$

$$= 0.2186x10^4 m/s$$

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

$$\lambda = \frac{6.626 \times 10^{-34}}{1.67 \times 410^{-27} \times 0.2186 \times 10^4}$$

=0.181nm

6. **Calculate the energies that can be possessed by a particle of mass 8.50 x10^{-31}kg which is placed in an infinite potential box of width 10^{-9}cm.[June 2012]**

Solution: The possible energies of a particle in an infinite potential box of width L is given by $E_n = \frac{n^2h^2}{8mL^2}$

M=8.50 x 10^{-31}Kg

L=1 x 10^{-11}m

h=6.626× 10^{-34}J-s

For ground state n=1

$$E_1 = \frac{6.626 X 10^{-34}}{8(8.50 \times 10^{-31})(1 \times 10^{-11})^2}$$

$$=6.456 \times 10^{-16} \text{ joule}$$

For first excited state $E_2 = 4 \times 6.4456 \times 10^{-16}$

$= 258.268 \times 10^{-16}$ Joule

7. **Calculate the wavelength of matter wave associated with a neutron whose kinetic energy is 1.5times the rest mass of electron.[Given that mass of neutron=1.676×10^{-27}kg,mass of electron 9.1×10^{-31}Kg,Mass of electron 9.1×10^{-31}J-Sec,velocity of light is 3×10^{8}m/s](June 2010,set1).**

Solution: For neutron $\frac{1}{2}m\upsilon^2 = 1.5\times9.1\times10^{-31}$ Joules

Or $$\upsilon^2 = \frac{2(1.5 \times 9.1\times10^{-31})}{1.676 \times 10^{-27}}$$

$$= 16.288\times10^{-4}$$

$$\upsilon = \sqrt{16.288 \times 10^{-4}}$$

$$= 4.046 \times10^{-2} \text{m/s}$$

The de-Broglie wavelength expression is

$$\lambda = \frac{h}{m\upsilon}$$

$$= \frac{6.62\times10^{-34}}{1.676\ X\ 10^{-2} \times 4.046X10^{-2}}$$

$$= 9.76X10^{-6}\text{m}$$

Questions

1) Drive Schrodinger's wave equation for the motion of an electron
2) describe the experimental verification of matter waves using Davisson-Germen experiment
3) Derive an expression for the de-Broglie wavelength of an electron
4) What are the important conclusions of G.P Thomson's experiment

(Or)

Describe the experimental verification of matter waves using G.P Thomson experiment
7) Write the physical significance of wave function
8) Write short notes on:
   i)De Broglie wavelength and
   ii)Heisenberg's uncertainty principle
9) What are matter waves? Derive an expression for the wavelength of matter waves
10) Describe an experiment to establish the wave nature of electron
11) Show that the energies of a particle in a potential box are quantized .

2.6 Analysis of Matter Wave or de-Broglie Wave

de-Broglie's suggestion that with any moving material particle there is a wave associated with it brings the problem of reconciliation of the two seemingly different manifestation of energy, that is, particle having mass which is localized in space and time while waves being massless are de-localized in space and time. The two possible solutions are either to de-localize the particle (no existing theory suggest it) or to localize a wave which is quite plausible using Principle of Superposition which suggests that it is possible to create waves of almost any shape (wave packet) by adding sine waves with properly chosen wave numbers (k), amplitudes and phases.

Further, while deriving the expression for velocity of de-Broglie wave, we will show a contradiction and thus led towards the idea that material particle cannot be equivalent to a single wave.

Let m be the mass of the particle and v be its velocity. Then

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

Also we have

$$E = mc^2 \text{ and } E = h\upsilon \quad \Rightarrow \upsilon = mc^2/h$$

Matter wave or de-Broglie wave velocity is

$$u = \nu\,\lambda = (mc^2/h)(h/mv) = c^2/v$$

Clearly for any material particle if $v < c$, then $u > c$ which is highly unexpected. Physically it means de-Broglie wave associated with a particle would travel faster than the particle itself, which indicates that material particle cannot be equivalent to a single wave.

Utilizing these above facts, one can visualize how a wave (not a single wave but a wave packet) resembles a particle. In other words, material particle (de-Broglie wave) in motion is equivalent to a wave packet rather than a single wave.

Wave packets have two velocities:

1. Phase velocity, $v_p = \omega/k$, by which individual wave constituting the packet moves.
2. Group velocity, $v_g = d\omega/dk$, by which the packet itself moves.

Clearly since phase velocity v_p (earlier u) is always greater than c, it is group velocity by which the particle moves.

To show $v_g = v$ we have angular frequency

$$\omega = 2\pi\nu = \frac{2\pi mc^2}{h}$$

and propagation constant

$$k = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h}$$

of de-Broglie wave associated with a particle of rest mass m_0 and moving with velocity v. We also have

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

Hence,

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

Now

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

The group velocity is given as

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

Thus, a moving particle can be represented by a 'wave group' or 'wave packet'. Finally, the phase velocity v_p of the de-Broglie wave associated with a moving particle is given as

$$v_p = \frac{\omega}{k} = \frac{E/\hbar}{p/\hbar} = \frac{E}{p} \tag{2.10}$$

The total relativistic energy 'E' of a particle is given by

$$E = \sqrt{p^2c^2 + m_0^2c^4} \tag{2.11}$$

Substituting this value in Eq. (2.10), we have

$$v_p = \frac{\sqrt{p^2c^2 + m_0^2c^4}}{p} = \frac{pc\sqrt{1+\frac{m_0^2c^2}{p^2}}}{p}$$

But $p = h/\lambda$. Therefore,

$$v_p = c\sqrt{1+\left(\frac{m_0 c\lambda}{h}\right)^2} \tag{2.12}$$

This equation shows that the phase velocity of a wave associated with a moving particle is always greater than c and even in free space it is a function of λ.

2.7 Davisson and Germer Experiment

In order to confirm the de-Broglie hypothesis, Davisson and Germer performed an experiment in 1927 to observe the diffraction of electrons. From this experiment the wavelength of the diffracted electrons

2.9 Phase Velocity and Group Velocity

When plane waves of different wavelengths travel simultaneously in the same direction along a straight line through a dispersive medium (a medium in which the phase velocity of a wave depends on its wavelength), successive groups of the waves are produced. These wave groups are called 'wave packet'. *The velocity of each individual wave of a wave packet is known as phase velocity*. The phase velocity is also called 'wave velocity' or 'velocity of propagation'. It is denoted by v_p and defined as

$$v_p = \frac{\omega}{k}$$

where ω is the angular velocity and k is the propagation constant of the wave.

The average velocity through which the wave packet propagates in the medium is called group velocity (v_g). The group velocity may also be defined as the velocity with which the energy in the group is transmitted. However, the individual waves travel inside the group with their own velocities. Mathematically, group velocity is given by

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

2.9.1 Expression for Phase Velocity

A plane harmonic wave travelling along the positive x-direction is given by

$$y = a\sin(\omega t - kx) \tag{2.19}$$

where a is the amplitude, $\omega = 2\pi n$ is the angular frequency and $k = 2\pi/\lambda$ is the propagation constant.

By definition, the ratio of angular frequency ω to propagation constant k is wave velocity. Thus

$$v_p = \frac{\omega}{k} \tag{2.20}$$

In Eq. (2.19), $(\omega t - kx)$ is the phase of wave motion. Then the planes of constant phase (wave front) are defined as

$$\omega t - kx = \text{constant} \tag{2.21}$$

Differentiating w.r.t. t, we get

$$\omega - k\frac{dx}{dt} = 0 \Rightarrow \frac{dx}{dt} = \frac{\omega}{k}$$

but

$$\frac{dx}{dt} = v_p \quad \Rightarrow v_p = \frac{\omega}{k} \tag{2.22}$$

Equation (2.22) is the required expression for phase velocity.

2.9.2 Expression for Group Velocity

Let us consider a wave group which consists of two components of equal amplitude 'a' and slightly different angular frequencies ω_1 and ω_2 and propagation constants k_1 and k_2, respectively. Their separate displacement are given by

$$y_1 = a\sin(\omega_1 t - k_1 x) \tag{2.23}$$

$$y_2 = a\sin(\omega_2 t - k_2 x) \tag{2.24}$$

Using principle of superposition we have

$$y = y_1 + y_2 = a\,[\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)]$$

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

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

$$= 2a \cos\left[\frac{(\omega_1 - \omega_2)t}{2} - \frac{(k_1 - k_2)x}{2}\right]\sin\left[\frac{(\omega_1 + \omega_2)t}{2} - \frac{(k_1 + k_2)x}{2}\right] \tag{2.25}$$

Equation (2.25) represents a wave group of frequency $(\omega_1 + \omega_2)/2$ and amplitude

$$A = 2a \cos\left[\frac{(\omega_1 - \omega_2)t}{2} - \frac{(k_1 - k_2)x}{2}\right] \tag{2.26}$$

Thus, the amplitude of the wave group is modulated both in space and time by a very slowly varying envelope of frequency $(\omega_1 - \omega_2)/2$ and propagation constant $(k_1 - k_2)/2$. The maximum value of amplitude is $2a$. This envelope is represented by the dotted curve as shown in Fig. 4.

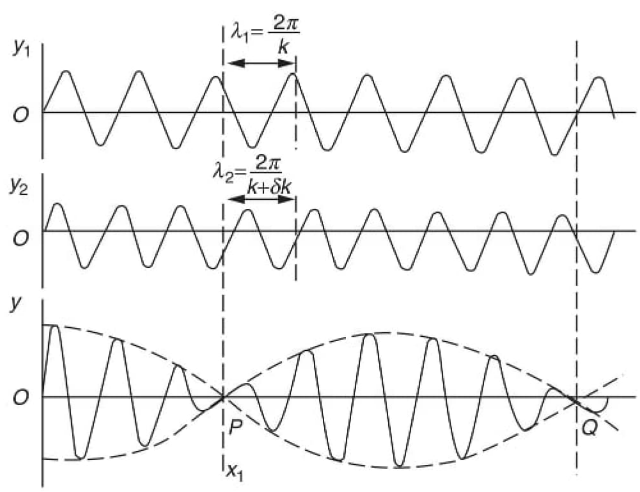

Figure 4 Modulation of wave.

The velocity with which this envelope advances, that is, the velocity of maximum amplitude of the group is given by

$$v_g = \frac{\omega_1 - \omega_2}{k_1 - k_2} = \frac{\Delta\omega}{\Delta k} \tag{2.27}$$

For infinitesimally small frequency interval, we can write

$$v_g = \frac{d\omega}{dk} \tag{2.28}$$

Equation (2.28) is the expression for group velocity.

2.9.3 Relation between Phase Velocity (v_p) and Group Velocity (v_g)

The group velocity is given by

$$v_{\text{g}} = \frac{d\omega}{dk} \tag{2.29}$$

and the phase velocity is given by

$$v_{\text{p}} = \frac{\omega}{k} \tag{2.30}$$

or

$$\omega = kv_{\text{p}} \tag{2.31}$$

Substituting the value of ω in Eq. (2.29), we have

$$v_{\text{g}} = \frac{d(kv_{\text{p}})}{dk} = k\frac{dv_{\text{p}}}{dk} + v_{\text{p}}$$

But $k = 2\pi/\lambda$. This implies

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

Therefore,

$$v_{\text{g}} = v_{\text{p}} - \frac{2\pi}{\lambda}\frac{\lambda^2}{2\pi}\frac{dv_{\text{p}}}{d\lambda} \quad \Rightarrow v_{\text{g}} = v_{\text{p}} - \lambda\frac{dv_{\text{p}}}{d\lambda} \tag{2.32}$$

Equation (2.32) is the required expression. Equation (2.32) shows that $v_{\text{g}} < v_{\text{p}}$ when the medium is dispersive, that is, when v_{p} is the function of λ. If there is no dispersive medium, that is, waves of all the wavelengths travel with same speed then $dv_{\text{p}}/d\lambda = 0$. So, Eq. (2.32) gives $v_{\text{g}} = v_{\text{p}}$. This result holds for elastic waves in homogeneous medium and electromagnetic waves in vacuum.

2.10 Phase Velocity of de-Broglie Waves

Let ω be the angular frequency and k be the propagation constant of de-Broglie wave. Then the phase velocity v_{p} of this wave is given by

$$v_{\text{p}} = \frac{\omega}{k} \tag{2.33}$$

According to de-Broglie hypothesis, the energy E and momentum p of a particle is given by

$$E = \hbar\omega \quad \text{and} \quad p = \hbar k$$

So,

$$E/p = \omega/k \quad \text{or} \quad v_{\text{p}} = E/p \tag{2.34}$$

Let m be the relativistic mass of the particle and v be its velocity. Then

$$E = mc^2 \quad \text{and} \quad p = mv$$

So,

$$v_{\text{p}} = mc^2/mv \quad \text{or} \quad v_{\text{p}} = c^2/v \tag{2.35}$$

But the particle velocity v is always less than c. Therefore, the phase velocity v_{p} is always greater than c. This is an unexpected result. According to this result, the wave associated with the moving particle would travel much faster than the particle itself and would leave the particle far behind. This is nothing but the failure of wave description of the particle. Therefore, the phase velocity has no physical meaning and the particle in motion is always associated with a wave packet.