Manonmaniam Sundaranar University,
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OPEN AND DISTANCE LEARNING(ODL) PROGRAMMES
(FOR THOSE WHO JOINED THE PROGRAMMES FROM THE ACADEMIC YEAR 2023–2024)

III YEAR

B.Sc. Physics

Course Material

Relativity and Quantum Mechanics

Prepared
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COURSE: SIXTH SEMESTER – CORE-8 (B.Sc PHYSICS)

COURSE TITLE: RELATIVITY AND QUANTUM MECHANICS

UNIT-I : SPECIAL THEORY OF RELATIVITY: Frames of reference – Galilean Relativity – Postulates of special theory of relativity – Lorentz transformations – length contraction – time dilation – concept of simultaneity – variation of mass with velocity – Einstein's mass-energy relation – relativistic momentum – energy relation.

UNIT-II : FAILURE OF CLASSICAL PHYSICS: Black body radiation – Failure of Classical Physics to explain energy distribution in the spectrum of a black body – Planck's Quantum theory – Wein's distribution law – Rayleigh Jean's law. Photo Electric Effect – Difficulty with Classical Physics – Einstein's Photo Electric Equation – work function.

UNIT-III : CONCEPT OF MATTER WAVES: de Broglie's concept of matter waves – expression for de Broglie's wavelength – phase velocity – group velocity relationship. Heisenberg's Uncertainty Principle – Elementary proof of Heisenberg's uncertainty relations.

UNIT-IV : OPERATORS AND SCHRÖDINGER EQUATION: Postulates of quantum mechanics. Wave functions and its interpretation – linear operators – Eigenvalue – Hermitian operator – Properties of Hermitian operator – Commutator Algebra. SCHRÖDINGER EQUATION: Schrödinger's wave equation in time dependent form – Steady state Schrödinger's wave equation – extension to three dimensions.

UNIT-V : APPLICATIONS OF SCHRÖDINGER EQUATIONS: Particle in a one-dimensional box – Particle in a rectangular three-dimensional box. Simple harmonic oscillator – One dimensional simple harmonic oscillator in quantum mechanics – zero-point energy. Reflection at step potential – Transmission across a potential barrier – Barrier Penetration (tunnelling effect).

TEXT BOOKS

1. Modern Physics, R. Murugeshan, KiruthigaSivaprasath, S. Chand and Co., 17th Revised Edition, 2014.
2. Concepts of Modern Physics, A. Beiser, 6th Ed., McGraw-Hill, 2003.
3. Special Theory of Relativity, S.P. Puri, Pearson Education, India, 2013.
4. Quantum Mechanics, Ghatak and Loganathan, Macmillan Publications.
5. Quantum Mechanics – Satyaprakash and Swati Saluja, KedarNath Ram Nath and Co.

UNIT I

SPECIAL THEORY OF RELATIVITY

Frames of reference – Galilean Relativity – Postulates of special theory of relativity – Lorentz transformations – length contraction – time dilation – concept of simultaneity – variation of mass with velocity – Einstein's mass-energy relation – relativistic momentum – energy relation.

1.1 INTRODUCTION

Classical or Newtonian mechanics deals with the motions of bodies travelling at velocities that are very much less than the velocity of light. According to it, the three fundamental concepts of Physics, *viz.*, space, time and mass are all absolute and invariant.

Concept of space. Newton assumed that space is absolute and "exists in itself, without relation to anything external and remains unaffected under all circumstances". This means to say that the length of an object is independent of the conditions under which it is measured, such as the motion of the object or the experimenter.

Concept of time. According to Newton, time is absolute 'by its very nature flowing uniformly without reference to anything external'. Hence there is a universal time flowing at a constant rate, unaffected by the motion or position of objects and observers. This implies two things:

(1) The interval of time between two events has the same value for all observers, irrespective of their state of motion.

(2) If two events are simultaneous for an observer, they are simultaneous for all observers, irrespective of their state of motion, *i.e.*, *simultaneity is absolute.*

Concept of mass. In Newtonian mechanics,

(1) The mass of a body does not depend on the velocity of its motion.

(2) The mass of an isolated system of bodies does not change with any processes occurring within the system (*law of conservation of mass*).

1.2 FRAME OF REFERENCE

A system of co-ordinate axes which defines the position of a particle in two or three dimensional space is called a *frame of reference*. The simplest frame of reference is the familiar Cartesian system of co-ordinates, in which the position of the particle is specified by its three co-ordinates *x,y,z,* along the three perpendicular axes. In Fig. 1.1 we have indicated two observers *O* and *O'* and a particle *P*. These observers use frames of reference *XYZ* and *X' Y' Z',* respectively. If *O* and *O'* are at rest, they will observe the same motion of *P*. But if *O* and *O'* are in relative motion, their observation of the motion of *P* will be different.

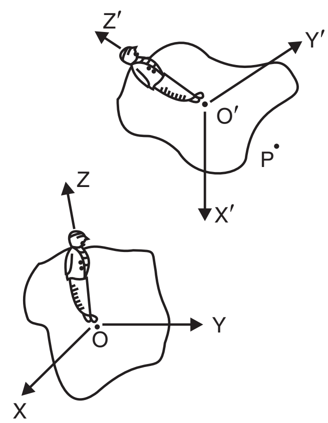


Fig. 1.1

Unaccelerated reference frames in uniform motion of translation relative to one another are called *Galilean frames or inertial frames.*

Accelerated frames are called *non-inertial* frames.

Definitions

(*i*) **Inertial frame of reference**

An *inertial frame of reference* is one in which Newton's first law of motion holds. In such a frame, an object at rest remains at rest and an object in motion continues to move at constant velocity (constant speed and direction) if no force acts on it. Any frame of reference that moves at constant velocity relative to an inertial frame is itself an inertial frame.

Special theory of relativity deals with the problems that involve inertial frames of reference.

(*ii*) **Non-inertial frame of reference**

A *non-inertial frame of reference* is the one in which the Newton's laws of motion are not valid *i.e.*, a body is accelerated when no external force acts on it.

1.3 NEWTONIAN PRINCIPLE OF RELATIVITY

Statement. *Absolute motion, which is the translation of a body from one absolute place to another absolute place, can never be detected. Translatory motion can be perceived only in the form of motion relative to other material bodies.*

Explanation: This implies that if we are drifting along at a uniform speed in a closed spaceship, all the phenomena observed and all the experiments performed inside the ship will appear to be the same as if the ship were not in motion. This means that the fundamental physical laws and principles are identical in all inertial frames of reference. This is the concept of Newtonian relativity.

1.4 GALILEAN TRANSFORMATION EQUATIONS

Let S and S' be two inertial frames (Fig. 1.2).

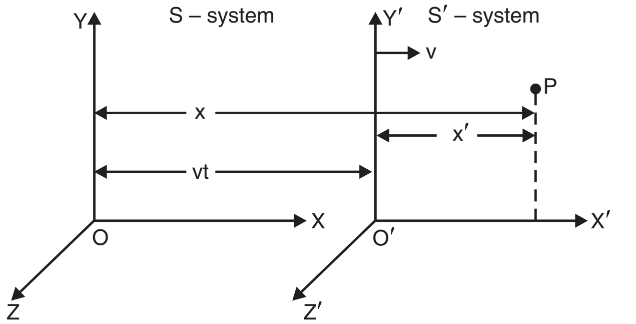


Fig. 1.2

Let S be at rest and S' move with uniform velocity v along the positive X direction. We assume that $v << c$. Let the origins of the two frames coincide at $t = 0$. Suppose some event occurs at the point P. The observer O in frame S determines the position of the event by the coordinates x, y, z. The observer O' in frame S' determines the position of the event by the coordinates x', y', z'. There is no relative motion between S and S' along the axes of Y and Z. Hence we have $y = y'$ and $z = z'$. Let the time proceed at the same rate in both frames.

The distance moved by S' in the positive X-direction in time $t = vt$. So the X coordinates of the two frames differ by vt. Hence, $x' = x - vt$.

Then the transformation equations from S to S' are given by,

$$x' = x - vt \; ... (1) \qquad y' = y \; ... (2) \qquad z' = z \; ... (3) \qquad t' = t \; ... (4)$$

Notes

(1) *The inverse transformation equations* (from S' to S) are

$$x = x' + vt, y = y', z = z' \text{ and } t = t'.$$

(2) In general, the transformation of velocities from one to the other system is obtained by taking time derivatives. When the relative motion of the two frames is confined to the X-direction, the transformation becomes,

$$\frac{dx'}{dt} = \frac{dx}{dt} - v \quad i.e., \quad u' = u - v; \; \frac{dy'}{dt} = \frac{dy}{dt}; \frac{dz'}{dt} = \frac{dz}{dt}.$$

(3) Let a and a' be the accelerations of the particle in S and S'. We have $a = \frac{du}{dt}$ and $a' = \frac{du'}{dt}$.

We have seen above that $u' = u - v$.

$$\therefore \quad \frac{du'}{dt} = \frac{du}{dt} \quad \text{(since } v \text{ is constant)}$$

or $a' = a$. *i.e., the accelerations, as measured by the two observers in the two frames, are the same.*

Hence we say that *acceleration is invariant under Galilean transformation.*

Assume that the velocity of the apparatus (or earth) relative to fixed ether is v in the direction PA. The relative velocity of a light ray travelling along PA is $(c - v)$ while its value would be $(c + v)$ for the returning ray. Let $PA = PB = d$.

Time taken by light to travel from P to $A = d/(c - v)$.

Time taken by light to travel from A to $P = d/(c + v)$.

∴ Total time taken by light to travel from P to A and back

$$t = \frac{d}{c-v} + \frac{d}{c+v} = \frac{2cd}{c^2 - v^2} = \frac{2d}{c}\left(1 + \frac{v^2}{c^2}\right) \qquad ...(1)$$

Now, consider the ray moving upwards from P to B. It will strike the mirror M_1 not at B but at B' due to the motion of the earth. If t_1 is the time taken by the ray starting from P to reach M_1, then $PB' = ct_1$ and $BB' = vt_1$.

The total path of the ray until it returns to $P = PB'P'$.

Now $PB'P' = PB' + B'P' = 2PB'$, since $PB' = B'P'$.

$$(PB')^2 = PC^2 + (CB')^2 = (BB')^2 + PB^2$$

i.e., $c^2t_1^2 = v^2t_1^2 + d^2$.

$$\therefore \quad t_1 = \frac{d}{\sqrt{c^2 - v^2}}$$

∴ Total time taken by the ray to travel the whole path $PB'P'$

$$\mathbf{t' = 2t_1 = \frac{2d}{\sqrt{c^2 - v^2}} = \frac{2d}{c\sqrt{1-(v^2/c^2)}} = \frac{2d}{c}\left(1 + \frac{v^2}{2c^2}\right)} \qquad ...(2)$$

Clearly, $t' < t$. The time difference

$$\Delta t = t - t' = \frac{2d}{c}\left(1 + \frac{v^2}{c^2}\right) - \frac{2d}{c}\left(1 + \frac{v^2}{2c^2}\right) = \frac{2d}{c} \times \frac{v^2}{2c^2} = \frac{dv^2}{c^3}.$$

The distance travelled by light in time $\Delta t = c \times \Delta t = dv^2/c^2$.

This is the path difference between the two parts of the incident beam. If the apparatus is turned through 90°, the path difference between the two beams becomes $2dv^2/c^2$. Michelson and Morley expected a fringe shift of about 0.4 in their apparatus when it was rotated through 90° and they believed that they could detect a shift as small as 0.01 of a fringe. But, in the experiment no displacement of the fringes was observed. They repeated the experiment at different points on the earth's surface and at different seasons of the year without detecting any measurable shift in fringes. *This negative result suggests that it is impossible to measure the speed of the earth relative to the ether.* Therefore, the effects of ether are undetectable. Thus, all attempts to make ether as a fixed frame of reference failed.

Explanation of the negative result. The negative result of the Michelson-Morley experiment can be explained by the following three explanations.

(1) The earth dragged along with it the ether in its immediate neighbourhood. Thus, there was no relative motion between the earth and ether. This is the explanation proposed by Michelson himself.

(2) Lorentz and Fitzgerald put forth the suggestion that there was contraction of bodies along the direction of their motion through the ether. Let L_0 be the length of the body when at rest. If it is moving with a speed v parallel to its length, the new length L is $L_0\sqrt{1-(v^2/c^2)}$. In the experiment

discussed above, the distance *PB* will remain unchanged. Distance *PA* will get shortened to $d\sqrt{1-(v^2/c^2)}$. If *d* were replaced by $d\sqrt{1-(v^2/c^2)}$ in equation (1), *t* and *t*′ will be the same and there will be no time difference expected. This contraction hypothesis easily explains why the Michelson-Morley experiment gave a negative result.

(3) The proper explanation for the negative result of the Michelson-Morley experiment was given by Einstein. He concluded that the velocity of light in space is a universal constant. This statement is called the *principle of constancy of the speed of light.* The speed of light is *c* rather than $|(c + v)|$ in any frame.

1.5 SPECIAL THEORY OF RELATIVITY

Einstein propounded the special theory of relativity in 1905. The special theory deals with the problems in which one frame of reference moves with a *constant linear velocity* relative to another frame of reference.

Postulates of special theory of relativity

(1) *The laws of Physics are the same in all inertial frames of reference.*

(2) *The velocity of light in free space is constant. It is independent of the relative motion of the source and the observer.*

***Explanation* :**

(1) The first postulate expresses the fact that, since it is impossible to perform an experiment which measures motion relative to a stationary ether, no unique stationary frame of reference can be discovered. Since there is no favoured 'rest' frame of reference, all systems moving with constant velocity must be on equal footing. We cannot discuss absolute motion. We can discuss only relative motion.

(2) We know that the velocity of light is not constant under Galilean transformations. But according to the second postulate, the velocity of light is the same in all inertial frames. Thus the second postulate is very important and only this postulate is responsible to differentiate the classical theory and Einstein's theory of relativity.

1.6 THE LORENTZ TRANSFORMATION EQUATIONS

We have to introduce new transformation equations which are consistent with the new concept of the invariance of light velocity in free space. The new transformation equations were discovered by Lorentz, and are known as "Lorentz transformations".

Derivation. Consider two observers *O* and *O'* in two systems *S* and *S*′. System *S*′ is moving with a constant velocity *v* relative to system *S* along the positive *X*-axis. Suppose we make measurements of time from the instant when the origins of *S* and *S*′ just coincide, *i.e.*, $t = 0$ when *O* and *O'* coincide. Suppose a light pulse is emitted when *O* and *O*′ coincide. The

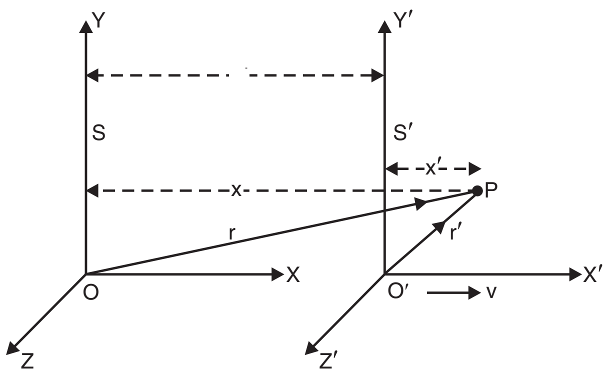


Fig. 1.3

light pulse produced at $t = 0$ will spread out as a growing sphere. The radius of the wave-front produced in this way will grow with speed c. After a time t, the observer O will note that the light has reached a point $P(x, y, z)$ as shown in Fig. 1.3. For him, the distance of the point P is given by $r = ct$. From figure, $r^2 = x^2 + y^2 + z^2$.

Hence, $$x^2 + y^2 + z^2 = c^2 t^2. \quad ...(1)$$

Similarly, the observer O' will note that the light has reached the same point P in a time t' with the same velocity c. So $r' = ct'$.

$\therefore$ $$x'^2 + y'^2 + z'^2 = c^2 t'^2 \quad ...(2)$$

Now, equations (1) and (2) must be equal since both the observers are at the centre of the same expanding wavefront.

$\therefore$ $$x^2 + y^2 + z^2 - c^2 t^2 = x'^2 + y'^2 + z'^2 - c^2 t'^2 \quad ...(3)$$

Since there is no motion in the Y and Z directions, $y' = y$ and $z' = z$.

$\therefore$ Equation (3) becomes,

$$x^2 - c^2 t^2 = x'^2 - c^2 t'^2 \quad ...(4)$$

The transformation equation relating to x and x' can be written as,

$$x' = k(x - vt) \quad ...(5)$$

Here, k is a constant.

The reason for trying the above relation is that, the transformation must reduce to Galilean transformation for low speed ($v << c$).

Similarly, let us assume that

$$t' = a(t - bx) \quad ...(6)$$

Here, a and b are constants.

Substituting these values for x' and t' in equation (4), we have,

$$x^2 - c^2 t^2 = k^2 (x - vt)^2 - c^2 a^2 (t - bx)^2$$

i.e., $$x^2 - c^2 t^2 = (k^2 - c^2 a^2 b^2)\, x^2 - 2(k^2 v - c^2 a^2 b)\, xt - \left(a^2 - \frac{k^2 v^2}{c^2}\right) c^2 t^2 \quad ...(7)$$

Equating the coefficients of corresponding terms in equation (7),

$$k^2 - c^2 a^2 b^2 = 1 \quad ...(8)$$

$$k^2 v - c^2 a^2 b = 0 \quad ...(9)$$

$$a^2 - \frac{k^2 v^2}{c^2} = 1 \quad ...(10)$$

Solving the above equations for k, a and b, we get,

$$k = a = \frac{1}{\sqrt{1 - (v^2/c^2)}} \quad ...(11)$$

and $$b = v/c^2 \quad ...(12)$$

Substituting these values of k, a and b in (5) and (6) we have,

$$x' = \frac{x - vt}{\sqrt{1 - (v^2/c^2)}} \text{ and } t' = \frac{t - (vx/c^2)}{\sqrt{1 - (v^2/c^2)}}$$

Therefore, the Lorentz transformation equations are

$$x' = \frac{x - vt}{\sqrt{1 - (v^2/c^2)}};\ y' = y;\ z' = z \text{ and } t' = \frac{t - (vx/c^2)}{\sqrt{1 - (v^2/c^2)}} \quad ...(13)$$

The inverse Lorentz transformation equations are obtained by interchanging the coordinates and replacing v by $-v$ in the above.

$$x = \frac{x' + vt'}{\sqrt{1-(v^2/c^2)}},\ y = y';\ z = z' \text{ and } t = \frac{t' + \left(vx'/c^2\right)}{\sqrt{1-\left(v^2/c^2\right)}} \quad ...(14)$$

These equations convert measurements made in frame S' into those in frame S.

Example 1. *Show that for values of $v << c$, Lorentz transformation reduces to the Galilean transformation.*

Sol. When $v << c$, $\frac{v}{c} \longrightarrow 0$; $\therefore \frac{1}{\sqrt{1-(v^2/c^2)}} \approx 1.$

We have from (13), $x' = x - vt$; $y' = y$; $z' = z$ and $t' = t$
which are Galilean transformations.

Example 2. *Show that if (x_1, y_1, z_1, t_1) and (x_2, y_2, z_2, t_2) are the coordinates of one event in S_1 and the corresponding event in S_2 respectively, then the expression*

$$ds_1^2 = dx_1^2 + dy_1^2 + dz_1^2 - c^2\,dt_1^2$$

is invariant under a Lorentz transformation of coordinates.

Sol. The inverse Lorentz transformation equations are:

$$x_1 = \frac{x_2 + vt_2}{\sqrt{1-\beta^2}};\ y_1 = y_2;\ z_1 = z_2 \text{ and } t_1 = \frac{t_2 + vx_2/c^2}{\sqrt{1-\beta^2}} \quad \text{(where } v/c = \beta\text{)}.$$

Differentiating,

$$dx_1 = \frac{dx_2 + v\,dt_2}{\sqrt{1-\beta^2}};\ dy_1 = dy_2;\ dz_1 = dz_2 \text{ and } dt_1 = \frac{dt_2 + (\beta/c)\,dx_2}{\sqrt{1-\beta^2}}$$

$$ds_1^2 = \left(\frac{dx_2 + v\,dt_2}{\sqrt{1-\beta^2}}\right)^2 + dy_2^2 + dz_2^2 - c^2\left(\frac{dt_2 + (\beta/c)\,dx_2}{\sqrt{1-\beta^2}}\right)^2$$

This simplifies to

$$ds_1^2 = dx_2^2 + dy_2^2 + dz_2^2 - c^2\,dt_2^2 = ds_2^2$$

1.7 LENGTH CONTRACTION

Consider two coordinate systems S and S' with their X-axes coinciding at time $t = 0$. S' is moving with a uniform relative speed v with respect to S in the positive X-direction. Imagine a rod (AB), at rest relative to S' (Fig. 1.4).

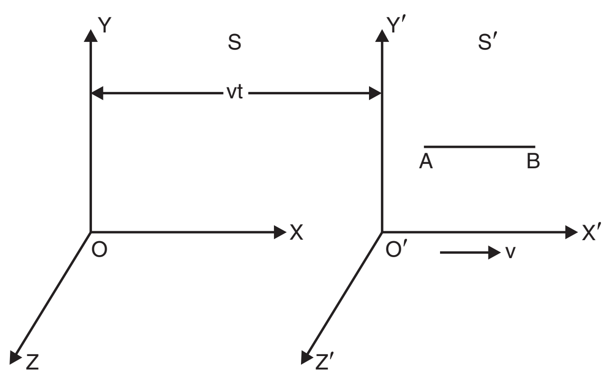


Fig. 1.4

Let x'_1 and x'_2 be the coordinates of the ends of the rod at any instant of time in S'. Then,

$$l_0 = x_2' - x_1' \quad ...(1)$$

since the rod is at rest in frame S'.

Similarly, let x_1 and x_2 be the

coordinates of the ends of the rod at the same instant of time in S.

Then $$l = x_2 - x_1 \quad ...(2)$$

l is the length of the rod, measured relative to S.

According to Lorentz transformations,

$$x_2' = \frac{x_2 - vt}{\sqrt{1-(v^2/c^2)}} \quad ...(3)$$

and $$x_1' = \frac{x_1 - vt}{\sqrt{1-(v^2/c^2)}} \quad ...(4)$$

Subtracting equation (4) from (3)

$$x_2' - x_1' = \frac{x_2 - x_1}{\sqrt{1-(v^2/c^2)}} \quad \text{or} \quad l_0 = \frac{l}{\sqrt{1-(v^2/c^2)}}$$

$$\therefore \quad l = l_0\sqrt{1-(v^2/c^2)} \quad ...(5)$$

From equation (5) we see that $l < l_0$. Therefore, to the observer in S it would appear that the length of the rod (in S') has contracted by the factor $\sqrt{1-(v^2/c^2)}$.

For example, a body which appears to be spherical to an observer at rest relative to it, will appear to be an oblate spheroid to a moving observer. Similarly, a square and a circle in one appear to the observer in the other to be a rectangle and an ellipse respectively (Fig. 1.5).

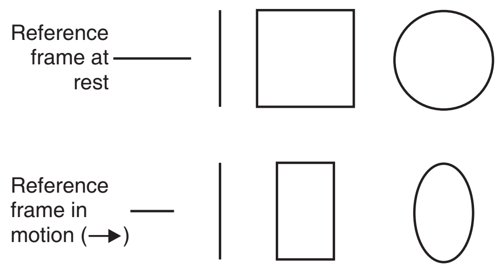


Fig. 1.5

Notes

(1) The *proper length* of an object is the length determined by an observer at rest with respect to the object. In the above case, l_0 is the proper length.

(2) The shortening or contraction in the length of an object along its direction of motion is known as the Lorentz-Fitzgerald contraction. There is no contraction in a direction perpendicular to the direction of motion.

(3) The contraction becomes appreciable only when $\mathbf{v} \approx \mathbf{c}$.

(4) The contraction is reciprocal, *i.e.*, if two identical rods are at rest—one in S and the other in S', each of the observers finds that the other is shorter than the rod of his own system.

EXAMPLE 1. *A rod* 1 *metre long is moving along its length with a velocity* 0.6*c*. *Calculate its length as it appears to an observer* (*a*) *on the earth* (*b*) *moving with the rod itself.*

SOL. Here, 1 metre is the proper length (l_0) of the rod in its own moving frame of reference. (*a*) Let l be the length of the rod as it appears to an observer in the stationary reference frame of the earth.

Here, $\mathbf{l_0 = 1\ m;\ v = 0.6\ c;}\ \ l = ?$

$$l = l_0\sqrt{1-\frac{v^2}{c^2}} = 1\sqrt{1-\frac{(0.6c)^2}{c^2}} = 1\sqrt{1-0.36} = 0.8 \text{ m}$$

Hence, the observer on the earth will estimate the length of the rod to be 0.8 metre.

(*b*) For an observer moving with the rod itself, the length of the rod is 1 metre.

EXAMPLE 2. *How fast would a rocket have to go relative to an observer for its length to be contracted to 99% of its length at rest*?

SOL. Here, $l = 0.99 l_0; \quad v = ?$

We have,

$$l = l_0\sqrt{1-(v^2/c^2)}$$

$$l^2 = l_0^2\left(1-\frac{v^2}{c^2}\right) \text{ or } \left(1-\frac{v^2}{c^2}\right) = \frac{l^2}{l_0^2} \text{ or } \frac{v^2}{c^2} = 1-\frac{l^2}{l_0^2}.$$

$$\therefore \quad v^2 = c^2\left(1-\frac{l^2}{l_0^2}\right) = c^2\,(1-0.99^2)$$

$$\therefore \quad v = 0.1416\,c = 0.1416 \times (3 \times 10^8) = 4.245 \times 10^7 \text{ ms}^{-1}$$

1.8 TIME DILATION

Imagine a gun placed at the position (x', y', z') in S' (Fig. 1.6).

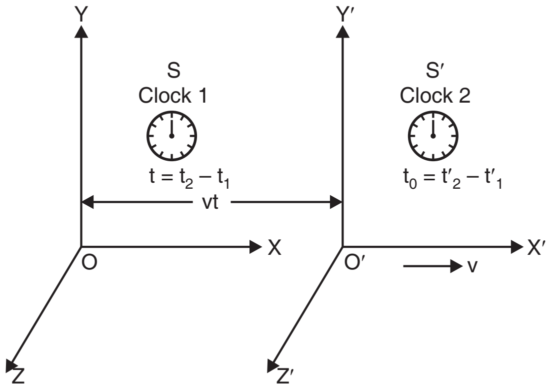


Fig. 1.6 A moving clock ticks more slowly than a clock at rest

Suppose it fires two shots at times t_1' and t_2' measured with respect to S'. In S' the clock is at rest relative to the observer. The time interval measured by a clock at rest relative to the observer is called the *proper time interval.* Hence, $t_0 = t_2' - t_1'$ is the time interval between the two shots for the observer in S'.

Since the gun is fixed in S', it has a velocity v with respect to S in the direction of the positive X-axis. Let $t = t_2 - t_1$ represent the time interval between the two shots as measured by an observer in S.

From inverse Lorentz transformations, we have

$$t_1 = \frac{t_1' + vx'/c^2}{\sqrt{1-(v^2/c^2)}} \quad \text{and} \quad t_2 = \frac{t_2' + vx'/c^2}{\sqrt{1-(v^2/c^2)}}$$

$$\therefore \quad t_2 - t_1 = \frac{t_2' - t_1'}{\sqrt{1-(v^2/c^2)}} \quad \text{or} \quad t = \frac{t_0}{\sqrt{1-(v^2/c^2)}}$$

$$\text{or} \quad t > t_0.$$

Thus, the time interval, between two events occurring at a given point in the moving frame S' appears to be longer to the observer in the stationary frame S; *i.e.*, a stationary clock measures a longer time interval between events occurring in a moving frame of reference than does a clock in the moving frame. This effect is called *time dilation.*

The Twin Paradox. Consider two exactly identical twin brothers. Let one of the twins go to a long space journey at a high speed in a rocket and the other stay behind on the earth. The clock in the moving rocket will appear to go slower than the clock on the surface of the earth (in accordance with $t = \dfrac{t_0}{\sqrt{1-(v^2/c^2)}}$). Therefore, when he returns back to the earth, he will find himself younger than the twin who stayed behind on the earth!

EXAMPLE 1. *A clock in a space ship emits signals at intervals of* 1 *second as observed by an astronaut in the space ship. If the space ship travels with a speed of* 3×10^7 *ms*$^{-1}$, *what is the interval between successive signals as seen by an observer at the control centre on the ground*?

SOL. Here, $t_0 = 1\text{s}$; $v = 3 \times 10^7\ \text{ms}^{-1}$; and $c = 3 \times 10^8\ \text{ms}^{-1}$; $t = ?$

$$\therefore \qquad t = \frac{t_0}{\sqrt{1-\dfrac{v^2}{c^2}}} = \frac{1}{\sqrt{1-\dfrac{(3\times 10^7)^2}{(3\times 10^8)^2}}} = 1.005\ \text{s}.$$

EXAMPLE 2. *A particle with a proper lifetime of* $1\mu s$ *moves through the laboratory at* $2.7 \times 10^8\ \text{ms}^{-1}$. (*a*) *What is its lifetime, as measured by observers in the laboratory*? (*b*) *What will be the distance traversed by it before disintegrating*?

SOL. Here, $t_0 = 1\mu s = 10^{-6}\text{s}$; $v = 2.7 \times 10^8\ \text{ms}^{-1}$; $t = ?$

$$(a) \qquad t = \frac{t_0}{\sqrt{1-\dfrac{v^2}{c^2}}} = \frac{10^{-6}}{\sqrt{1-\dfrac{(2.7\times 10^8)^2}{(3\times 10^8)^2}}} = 2.3 \times 10^{-6}\ \text{s}.$$

(*b*) The average distance moved by the particle before disintegration $= (2.7 \times 10^8) \times (2.3 \times 10^{-6})$
$= 620$ m.

1.9 RELATIVITY OF SIMULTANEITY

Consider two events—the explosion of a pair of time bombs—that occur at the same time to an observer *O* in a reference frame *S*. Let the two events occur at different locations x_1 and x_2. Consider another observer O' in S' moving with a uniform relative speed *v* with respect to *S* in the positive *X*-direction.

To O', the explosion at x_1 and t_0 occurs at the time

$$t'_1 = \frac{t_0 - (v/c^2)\,x_1}{\sqrt{1-(v^2/c^2)}}$$

and the explosion at x_2 and t_0 occurs at the time

$$t'_2 = \frac{t_0 - (v/c^2)\,x_2}{\sqrt{1-(v^2/c^2)}}$$

$\therefore$ The time interval between the two events as observed by the observer O'

$$= t' = t'_2 - t'_1 = \frac{(v/c^2)(x_1 - x_2)}{\sqrt{(1-v^2/c^2)}}$$

This is not zero. This indicates that two events at x_1 and x_2, which are simultaneous to the observer in *S*, do not appear so to the observer in S'. Therefore, the concept of simultaneity has only a relative and not an absolute meaning.

Notes

(1) This law of addition of velocities applies only when the two velocities are in the same direction.

(2) If $v << c$, we get the classical equation.

(3) We can express the velocity u' in terms of u and v.

$$u' = \frac{u-v}{1-\frac{uv}{c^2}}$$

Example 1. *An experimenter observes a radioactive atom moving with a velocity of* $0.25c$. *The atom then emits a* β *particle which has a velocity of* $0.9c$ *relative to the atom in the direction of its motion. What is the velocity of the* β *particle, as observed by the experimenter?*

Sol. Here, $v = 0.25c$; $u' = 0.9c$; $u = ?$

$$u = \frac{u'+v}{1+\frac{v}{c^2}u'} = \frac{0.9c+0.25c}{1+\frac{0.25c}{c^2}\times 0.9c} = 0.94c.$$

Example 2. *An electron is moving with a speed of* $0.85c$ *in a direction opposite to that of a moving photon. Calculate the relative velocity of the photon with respect to the electron.*

Sol. Let the photon be moving along the positive direction of X-axis and the electron along the negative direction of X-axis. Then, the speed of electron = – $0.85c$; the speed of photon = c.

Consider that the electron is at rest in system S. Then, we may assume that the system S' (laboratory) is moving with velocity $0.85c$ relative to system S (electron). *i.e.*, $v = 0.85c$; $u' = c$; $u = ?$

$$u = \frac{u'+v}{1+\frac{u'v}{c^2}} = \frac{c+0.85c}{1+\frac{(c)\times(0.85c)}{c^2}} = c.$$

1.10 VARIATION OF MASS WITH VELOCITY

Derivation. Consider two systems *S* and *S*′. *S*′ is moving with a constant velocity *v* relative to the system *S*, in the positive *X*-direction (Fig. 1.7). Suppose that in the system *S*′, two exactly similar elastic balls *A* and *B* approach each other at equal speeds (*i.e.*, *u* and –*u*). Let the mass of each ball be *m* in *S*′. They collide with each other and after collision coalesce into one body. According to the law of conservation of momentum,

Momentum of ball *A* + momentum of ball *B* = momentum of coalesced mass.

Or $mu + (-mu)$ = momentum of coalesced mass = 0.

Thus the coalesced mass must be at rest in *S*′ system.

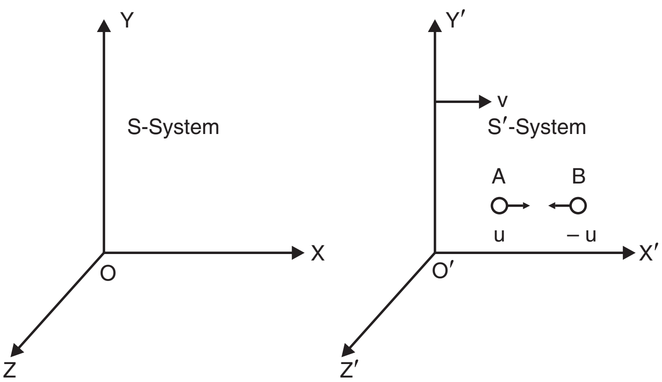


Fig. 1.7

Let us now consider the collision with reference to the system *S*.

Let u_1 and u_2 be the velocities of the balls relative to *S*. Then,

$$u_1 = \frac{u+v}{1+uv/c^2} \quad \text{...(1)}$$

and

$$u_2 = \frac{-u+v}{1-uv/c^2} \quad \text{...(2)}$$

After collision, velocity of the coalesced mass is *v* relative to the system *S*.

Let mass of the ball *A* travelling with velocity u_1 be m_1 and that of *B* with velocity u_2 be m_2 in the system *S*. Total momentum of the balls is conserved. Therefore,

$$m_1 u_1 + m_2 u_2 = (m_1 + m_2) v \quad \text{...(3)}$$

Substituting for u_1 and u_2 from equations (1) and (2), we have,

$$m_1 \left[\frac{u+v}{1+uv/c^2}\right] + m_2 \left[\frac{-u+v}{1-uv/c^2}\right] = (m_1 + m_2)v$$

or

$$m_1 \left[\frac{u+v}{1+\frac{uv}{c^2}} - v\right] = m_2 \left[v - \frac{-u+v}{1-\frac{uv}{c^2}}\right]$$

or $$m_1\left[\frac{u+v-v-uv^2/c^2}{1+uv/c^2}\right] = m_2\left[\frac{v-uv^2/c^2+u-v}{1-uv/c^2}\right]$$

or $$m_1\left[\frac{u\left(1-\frac{v^2}{c^2}\right)}{1+\frac{uv}{c^2}}\right] = m_2\left[\frac{u\left(1-\frac{v^2}{c^2}\right)}{1-\frac{uv}{c^2}}\right]$$

or $$\frac{m_1}{m_2} = \frac{1+uv/c^2}{1-uv/c^2} \qquad ...(4)$$

Also, $$1-\frac{u_1^2}{c^2} = 1-\frac{\left\{\frac{u+v}{c}\right\}^2}{\left(1+\frac{uv}{c^2}\right)^2}$$

$$= \frac{1+\frac{u^2v^2}{c^4}+\frac{2uv}{c^2}-\frac{u^2}{c^2}-\frac{v^2}{c^2}-\frac{2uv}{c^2}}{\left(1+\frac{uv}{c^2}\right)^2}$$

$$= \frac{\left(1-\frac{u^2}{c^2}\right)-\frac{v^2}{c^2}\left(1-\frac{u^2}{c^2}\right)}{\left(1+\frac{uv}{c^2}\right)^2}$$

$$1-\frac{u_1^2}{c^2} = \frac{\left(1-\frac{u^2}{c^2}\right)\left(1-\frac{v^2}{c^2}\right)}{\left(1+\frac{uv}{c^2}\right)^2} \qquad ...(5)$$

Similarly, $$1-\frac{u_2^2}{c^2} = \frac{\left(1-\frac{u^2}{c^2}\right)\left(1-\frac{v^2}{c^2}\right)}{\left(1-\frac{uv}{c^2}\right)^2} \qquad ...(6)$$

Dividing equation (6) by equation (5),

$$\frac{1-\frac{u_2^2}{c^2}}{1-\frac{u_1^2}{c^2}} = \frac{\left(1+\frac{uv}{c^2}\right)^2}{\left(1-\frac{uv}{c^2}\right)^2}$$

or $$\frac{\sqrt{1-\frac{u_2^2}{c^2}}}{\sqrt{1-\frac{u_1^2}{c^2}}} = \frac{1+\frac{uv}{c^2}}{1-\frac{uv}{c^2}} \qquad ...(7)$$

From equations (7) and (4), $$\frac{m_1}{m_2} = \frac{\sqrt{1-\frac{u_2^2}{c^2}}}{\sqrt{1-\frac{u_1^2}{c^2}}}$$

or $$m_1\sqrt{1-\frac{u_1^2}{c^2}} = m_2\sqrt{1-\frac{u_2^2}{c^2}} \qquad ...(8)$$

Since the L.H.S. and R.H.S. of equation (8) are independent of one another, the above result can be true only if each is a constant. Therefore,

$$m_1\sqrt{1-\frac{u_1^2}{c^2}} = m_2\sqrt{1-\frac{u_2^2}{c^2}} = m_0.$$

The constant denoted by m_0 is called the *rest mass* of the body and corresponds to *zero velocity.*

Thus, $$m_1 = \frac{m_0}{\sqrt{1-u_1^2/c^2}}$$

In general, if m denotes the mass of a body when it is moving with a velocity v, then,

$$m = \frac{m_0}{\sqrt{1-v^2/c^2}} \qquad ...(9)$$

This is the relativistic formula for the variation of mass with velocity.

If we put $v \to c$ in equation (9), we have $m \to \infty$ *i.e.*, an object travelling at the speed of light would have infinite mass. Thus, Eqn. (9) shows that no material body can have a velocity equal to, or greater than the velocity of light.

Notes

(1) The first verification of the increase in mass with velocity came from the work of Kaufmann in 1906 and of Bucherer in 1909. While studying the β-rays emanating from radioactive materials, they found that their velocities were comparable to the velocity of light and also that their masses were found to be related to their velocities.

(2) The increase of mass with velocity has now been tested in "*particle accelerators*". Accelerators are used to accelerate the various charged particles of matter to very high velocities. It has been found that the electrons and protons accelerated in these machines to velocities close to the velocity of light acquire increased masses, exactly as predicted.

Example. *At what speed is a particle moving if the mass is equal to three times its rest mass*?

Sol. We have, $$m = \frac{m_0}{\sqrt{1-v^2/c^2}}. \text{ Here, } m = 3m_0;\ v = ?$$

$$\therefore \quad 3m_0 = \frac{m_0}{\sqrt{1-v^2/c^2}} \text{ or } \sqrt{1-\frac{v^2}{c^2}} = \frac{1}{3} \text{ or } 1-\frac{v^2}{c^2} = \frac{1}{9}$$

Or $$\frac{v^2}{c^2} = \frac{8}{9} \text{ or } v^2 = \frac{8}{9}c^2 \text{ or } v = \sqrt{\frac{8}{9}}c = 0.94c.$$

1.11 MASS ENERGY EQUIVALENCE

Derivation. Force is defined as rate of change of momentum *i.e.*,

$$F = \frac{d}{dt}(mv) \qquad ...(1)$$

According to the theory of relativity, both mass and velocity are variable. Therefore,

$$F = \frac{d}{dt}(mv) = m\frac{dv}{dt} + v\frac{dm}{dt} \qquad \text{...(2)}$$

Let the force F displace the body through a distance dx.

Then, the increase in the kinetic energy (dE_k) of the body is equal to the work done ($F\,dx$).

Hence, $$dE_k = F\,dx = m\frac{dv}{dt}dx + v\frac{dm}{dt}dx$$

or $$dE_k = mv\,dv + v^2\,dm \qquad \text{...(3)}$$

According to the law of variation of mass with velocity

$$m = \frac{m_0}{\sqrt{(1 - v^2/c^2)}} \qquad \text{...(4)}$$

Squaring both sides, $$m^2 = \frac{m_0{}^2}{1-(v^2/c^2)}$$

or $$m^2 c^2 = m_0^2 c^2 + m^2 v^2$$

Differentiating, $$c^2\, 2m\,dm = m^2\, 2v\,dv + v^2\, 2m\,dm$$

or $$c^2\,dm = mv\,dv + v^2\,dm \qquad \text{...(5)}$$

From equations (3) and (5), $$dE_k = c^2\,dm \qquad \text{...(6)}$$

Thus, a change in K.E. dE_k is directly proportional to a change in mass dm.

When a body is at rest, its velocity is zero, (K.E. = 0) and $m = m_0$. When its velocity is v, its mass becomes m. Therefore, integrating equation (6),

$$E_k = \int_o^{E_k} dE_k = c^2 \int_{m_o}^{m} dm = c^2(m - m_0)$$

$$\therefore \quad E_k = mc^2 - m_o c^2 \qquad \text{...(7)}$$

This is the relativistic formula for K.E.

When the body is at rest, the internal energy stored in the body is m_0c^2. m_0c^2 is called the rest mass energy. The total energy (E) of the body is the sum of K.E. (E_k) and rest mass energy (m_0c^2).

$$\therefore \quad E = E_k + m_0c^2 = (mc^2 - m_0c^2) + m_0c^2 = mc^2.$$

$$\therefore \quad E = mc^2$$

This is Einstein's mass-energy relation.

Notes

(1) This relation states a universal equivalence between mass and energy. It means that mass may appear as energy and energy as mass.

Example. Consider the phenomenon of pair-annihilation or pair production. In this phenomenon, an electron and a positron can combine and literally disappear. In their place we find high energy radiation called γ-radiation, whose radiant energy is exactly equal to the rest mass plus kinetic energies of the disappearing particles. The process is reversible, so that a materialization of mass from radiant energy can occur when a high enough energy γ-ray, under proper conditions, disappears. In its place appears a positron-electron pair whose total energy (rest mass + K.E.) is equal to the radiant energy lost.

(2) The relationship ($E = mc^2$) between energy and mass forms the basis of understanding nuclear reactions such as *fission* and *fusion*. These reactions take place in nuclear bombs and reactors. When a uranium nucleus is split up, the decrease in its total rest mass appears in the form of an equivalent amount of K.E. of its fragments.

(3) The formula for K.E. reduces to the classical formula for $v << c$.

$$E_k = mc^2 - m_0c^2 = (m - m_0)c^2 = m_0 c^2 [(1 - v^2/c^2)^{-1/2} - 1]$$

Now, since $v << c, \left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}} = 1 + \frac{v^2}{2c^2} + ...$ (neglecting higher order terms).

$$\therefore \quad E_k = m_0c^2 \times \frac{v^2}{2c^2} = \frac{1}{2} m_0 v^2.$$

Unified mass unit. The basic mass unit used in Atomic Physics is called the unified mass unit (u). It is defined as (1/12)th of the rest mass of carbon—12 atom. Thus, $1u = 1.66 \times 10^{-27}$ kg.

Now, $E = m_0 c^2 = (1.66 \times 10^{-27})(3 \times 10^8)^2 = 1.49 \times 10^{-10}$ J.

$$= \frac{1.49 \times 10^{-10}}{1.6 \times 10^{-19}} eV = 931.3 \text{ MeV}.$$

Hence the energy equivalent to unified mass unit is 931 MeV.

Example 1. *If 4 kg of a substance is fully converted into energy, how much energy is produced?*

Sol. Here, $m = 4$ kg, $c = 3 \times 10^8$ ms^{-1}; $E = ?$

$$E = mc^2 = 4 \times (3 \times 10^8)^2 = 3.6 \times 10^{17} \text{ J}.$$

Example 2. *Calculate the rest energy of an electron in joules and in electron volts.*

Sol. Here, m_0 = rest mass of the electron = 9.11×10^{-31} kg;

$$c = 3 \times 10^8 \text{ ms}^{-1}$$

$$\therefore \quad E = m_0c^2 = (9.11 \times 10^{-31})(3 \times 10^8)^2 = 8.2 \times 10^{-14} \text{ J}.$$

$$= \frac{8.2 \times 10^{-14}}{1.6 \times 10^{-19}} eV \quad (\text{since } 1eV = 1.6 \times 10^{-19} J).$$

$$= 0.51 \text{ MeV [mega electron volt]}.$$

Example 3. *Calculate the K.E. of an electron moving with a velocity of* 0.98 *times the velocity of light in the laboratory system.*

Sol. Relativistic formula for K.E. is $T = (m - m_0)c^2$.

Here, m_0 = rest mass of electron = 9.11×10^{-31} kg.

$c = 3 \times 10^8$ ms^{-1}; $v = 0.98c$.

We can find m using the formula

$$m = \frac{m_0}{\sqrt{(1 - v^2/c^2)}} = \frac{m_0}{\sqrt{1 - (0.98c/c)^2}} = 5.02\, m_0$$

$$\therefore \quad \text{K.E.} = (5.02\, m_0 - m_0)c^2 = 4.02\, m_0c^2$$

$$= 4.02 \times (9.11 \times 10^{-31})(3 \times 10^8)^2 = 3.296 \times 10^{-13} J.$$

1.11.1. Relationship Between the Total Energy, the Rest Energy, and the Momentum

The total relativistic energy (rest mass plus kinetic) of a particle is

$$E = mc^2 = m_0c^2 / (1 - v^2/c^2)^{1/2} \qquad ...(1)$$

The momentum of the particle is $p = mv$

or $\quad v = p/m.$ ...(2)

$$\therefore \quad E = m_0 \frac{c^2}{\sqrt{[1-(p^2/m^2c^2)]}} = \frac{m_0c^2}{\sqrt{[1-(p^2c^2/m^2c^4]}} = m_0 \frac{c^2}{\sqrt{[1-(p^2c^2/E^2)]}}$$

or $\quad E^2 = m_0^2 \dfrac{c^4}{(1-p^2c^2/E^2)}$ or $E^2 - p^2c^2 = m_0^2c^4$

$$\therefore \quad E^2 = m_0^2 c^4 + p^2c^2 \qquad ...(3)$$

1.11.2 Massless Particles

- In classical mechanics, a particle must have rest mass in order to have energy and momentum.
- But in relativistic mechanics, this requirement does not hold.

A particle can exist which has no rest mass but which exhibits such particlelike properties as energy and momentum. Relativistic momentum of a particle,

$$p = \frac{m_0v}{\sqrt{(1-v^2/c^2)}} \qquad ...(1)$$

Total energy of a particle,

$$E = \frac{m_0c^2}{\sqrt{1-v^2/c^2}} \qquad ...(2)$$

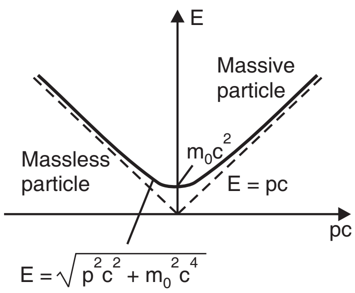


Fig. 1.8

From Eqs. (1) and (2), when $m_0 = 0$ and $v << c$, it is clear that $E = p = 0$.

A massless particle with a speed less than that of light can have neither energy nor momentum.

However when $m_0 = 0$ and $v = c$, $E = 0/0$ and $p = 0/0$, which are indeterminate: E and p can have any values. Thus Eqs. (1) and (2) are consistent with the existence of massless particles that possess energy and momentum *provided that they travel with the speed of light*.

The relationship between E, m_0c^2 and p is

$$E = \sqrt{(pc)^2 + (m_0c^2)^2} \qquad ...(3)$$

- For a massless particle with $m_0 = 0$:

$$E = pc \qquad ...(4)$$

Fig. 1.8 shows the relativistic energy as a function of momentum for massive and massless particles.

The conclusion is not that massless particles necessarily occur, only that the laws of physics do not exclude the possibility as long as $v = c$ and $E = pc$ for them. In fact, a massless particle—the photon—indeed exists and its behavior is as expected.

1.14.3 To show that the Rest Mass of a Photon is Zero

A photon travels with the velocity of light. Hence we must use the relativistic expression for its momentum, p.

Thus, for a photon

$$p = \frac{m_0v}{\sqrt{[1-(v^2/c^2)]}} \qquad ...(1)$$

Here, m_0 is the rest mass and v the velocity of the photon.

From quantum theory of radiation, the momentum of a photon of radiation of wavelength λ is

$$p = h/\lambda \qquad ...(2)$$

Here, h is the Planck's constant.

$$\therefore \qquad \frac{h}{\lambda} = \frac{m_0 v}{\sqrt{[1-(v^2/c^2)]}} \qquad ...(3)$$

or

$$m_0 = \frac{h}{v\lambda}\sqrt{[1-(v^2/c^2)]}\,.$$

Since for photon, $v = c$, we have

$$m_0 = 0.$$

Hence the rest mass of photon is zero.

EXERCISES

Part A: Choose the Correct Answer

1. The length of the rod moving with a velocity v relative to the observer at rest is contracted by a factor

(*a*) $\sqrt{1-\frac{v^2}{c^2}}$ (*b*) $\sqrt{1+\frac{v^2}{c^2}}$ (*c*) $\sqrt{1-\frac{c^2}{v^2}}$ (*d*) $\sqrt{1+\frac{c^2}{v^2}}$

2.

(*a*) $m = \frac{m_0}{\sqrt{1-\frac{v}{c}}}$ (*b*) $m = \frac{m_0}{\left(1-\frac{v}{c}\right)}$ (*c*) $m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$ (*d*) $m = \frac{m_0}{\sqrt{1+\frac{v^2}{c}}}$

3. Mass – Energy relation $E =$ ——————

(*a*) mc (*b*) mc^2 (*c*) m^2c (*d*) m^2c^2

4. The total relativistic energy is

(*a*) $E = c\sqrt{p^2 + m_0^2c^2}$ (*b*) $E = c\sqrt{p^2 - m_0^2c^2}$ (*c*) $E = c\sqrt{p^2 + m_0c^2}$ (*d*) $E = c\sqrt{p^2 - m_0c^2}$

5. The rest mass of photon is

(*a*) positive (*b*) finite (*c*) infinite (*d*) zero

Ans. **1.** (*a*), **2.** (*c*), **3.** (*b*), **4.** (*a*), **5.** (*d*).

Part B: Short Answer Questions

6. What is meant by frame of reference? Define inertial and non-inertial frames.

7. Explain Ether hypothesis.

8. State and explain the postulates of special theory of relativity.

9. Explain relativistic length contraction.

10. Explain the relativistic time dilation.

11. What is twin paradox?

12. If a particle could move with the velocity of light, how much kinetic energy would it possess?

[**Ans.** Since the mass of the particle moving with the velocity of light $\left(m = \frac{m_0}{\sqrt{1-v^2/c^2}}\right)$ becomes infinite, the kinetic energy would be also infinite. But it is impossible.]

14. Define unified mass unit and find its energy equivalence.

15. A particle of rest mass m_0 moves with speed $c/\sqrt{2}$. Calculate its mass, momentum, total energy and kinetic energy.

[**Hint.** (*i*) $m = \frac{m_0}{\sqrt{1-v^2/c^2}} = \frac{m_0}{\sqrt{1-\frac{1}{2}}} = 1.41\, m_0$

(*ii*) $p = mv = \sqrt{2}\, m_0 \times c/\sqrt{2} = m_0c$

(*iii*) $E = mc^2 = 1.41\, m_0c^2$.

(*iv*) K.E. $= E - m_0c^2 = 0.41\, m_0c^2$.]

16. What is the General Theory of Relativity? Discuss the important conclusions derived from it. What are the experimental observations in favour of these conclusions?

17. Is a laboratory at rest on the earth's surface really an inertial frame of reference?

[**Ans.** *No, because it is accelerated as a consequence of the earth's rotation on its axis and revolution around the sun*].

18. An astronomer on earth flashes a pulsed laser, and 1.3 sec. later the pulse reaches the moon 3.9×10^8 m away. An observer travelling in the same direction as the pulse sees the two events (*i.e.*, the flash and the arrival at the moon) as one event. What is the speed of this observer?

[**Ans.** *The observer must be moving at the speed of light in the same direction as the pulse.*]

19. Does the mass of a substance increase on melting? Why?

[**Ans.** *Yes. Because an amount of energy equal to the specific latent heat of fusion has been added to the substance.*]

20. If photons have a speed *c* in one reference frame, can they be found at rest in any other frame?

[**Ans.** *No. When a body moves with a speed less than c in one reference frame, we can find another reference frame in which it is at rest. But when the body moves with speed c in one reference frame, it will move with the same speed c in all reference frames*].

Part C: Long Answer Questions

21. Derive the Lorentz space-time transformation formula. Discuss the length contraction and time dilation.

22. Deduce the formula for relativistic variation of mass with velocity. Briefly explain its significance.

23. What is the meaning of mass-energy equivalence? Obtain Einstein's mass energy relation. Show that 1 amu = 931 MeV.

UNIT II

FAILURE OF CLASSICAL PHYSICS

Black body radiation – Failure of Classical Physics to explain energy distribution in the spectrum of a black body – Planck's Quantum theory – Wein's distribution law – Rayleigh Jean's law. Photo Electric Effect – Difficulty with Classical Physics – Einstein's Photo Electric Equation – work function.

2.1 Black Body Radiation

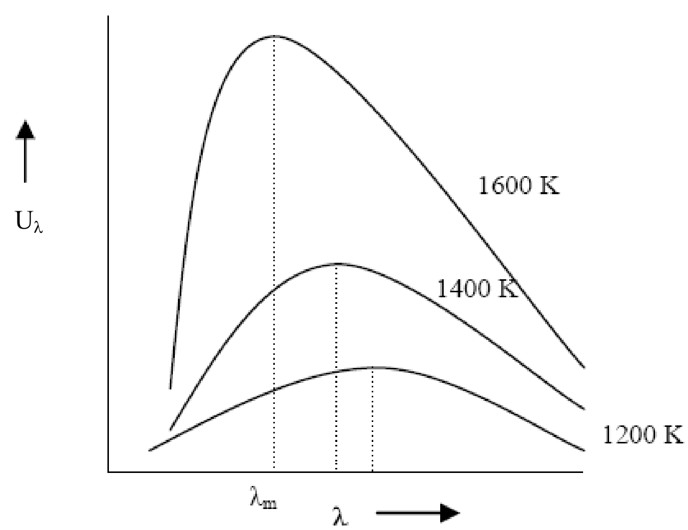
A hot body emits thermal radiations which depend on composition and the temperature of the body. The ability of the body to radiate is closely related to its ability to absorb radiation. A Body which is capable of absorbing almost all the radiations incident on it is called a black body. A perfectly black-body can absorb the entire radiations incident on it. Platinum black and Lamp black can absorb almost all the radiations incident on them.

Emissive power of a black body: It is defined as the total energy radiated per second from the unit surface area of a black body maintained at certain temperature.

Absorptive power of a black body: It is defined as the ratio of the total energy absorbed by the black body to the amount of radiant energy incident on it in a given time interval. The absorptive power of a perfectly black body is 1.

Spectral Distribution of energy in thermal radiation (Black Body radiation spectrum)

A good absorber of radiation is also a good emitter. Hence when a black body is heated it emits radiations. In practice a black body can be realized with the emission of Ultraviolet, Visible and infrared wavelengths on heating a body. German physicists Lummer and Pringsheim studied the energy density as a function of wavelength for different temperatures of a black body using a spectrograph and a plot is made. This is called Black Body radiation spectrum.



The Salient features of black body radiation spectrum are as below

1) The energy density increases with wavelength then takes a maximum value E_m for a particular wavelength λ_m and then decrease to a value zero for longer wavelengths. Hence the Energy distribution in the spectrum is not uniform
2) As the Temperature increases the Wavelength (λ_m) corresponding to the maximum emission energy (E_m) shifts towards shorter wavelength side. Thus the λ_m is inversely proportional to temperature (T) and is called **Wein's Displacement Law**. Mathematically $\lambda_m = \frac{b}{T}$ .Here b is Wein's Constant of value 2.898×10^{-3} mK.
3) The total energy emitted by the black body at a given temperature is given by the area under the curve and is proportional to the fourth power of temperature. This is called Stefan's law of radiation. Mathematically $E = \sigma T^4$, here 'σ' is the Stefan's constant of value 5.67×10^{-8} Wm^2K^{-4}.

Explanation of Black Body Radiation Spectrum

Classical Theories

Wein's Distribution Law: In the year 1893 Wein using thermodynamics showed that the energy emitted per unit volume in the wavelength range λ and $\lambda + d\lambda$

$$E_\lambda d\lambda = \frac{C_1}{\lambda^5} e^{-\frac{C_2}{\lambda T}} d\lambda$$

Here C_1 and C_2 are empirical constants. A suitable selection for these constants helps to explain the experimental curve in the shorter wavelength region. The drawback of this law is it fails to explain the curve in the longer wavelength region. Also according to this equation the energy density at high temperatures tends to zero which contradicts experimental observations.

Rayleigh-Jeans Law: British Physicists Lord Rayleigh and James Jeans made an attempt to explain the Black Body radiation spectrum Based on the concepts formation of standing electromagnetic waves and the law of equipartition of energy. According to this law the energy density of radiation is given by

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

Here 'k' is Boltzmann constant with value 1.38×10^{-23} JK^{-1}. This law successfully explains the energy distribution of the black body radiation in the longer wavelength region. According to this law black body is expected to radiate large amount of energy in the shorter wavelength region thus leading to no energy available for emission in the longer wavelength region. Experimental observations show that the most of the emissions of the black body radiation occur in the visible and infrared regions. This discrepancy is called **Ultraviolet Catastrophe**.

2.2 INADEQUACY OF CLASSICAL MECHANICS

Classical mechanics failed to explain the following phenomena:

(*i*) It does not hold in the region of atomic dimensions, *i.e.*, it can not explain the non-relativistic motion of atoms, electrons, protons etc.

- It could not explain the **stability of atoms**.
- It could not explain the origin of discrete spectra of atoms since, according to *classical mechanics, the energy changes are always continuous*.

(*ii*) It could not explain observed spectrum of black body radiation.

(*iii*) Classical mechanics could not explain observed phenomea like photoelectric effect, Compton effect etc.

(*iv*) It could not explain the observed variation of specific heat capacity of solids.

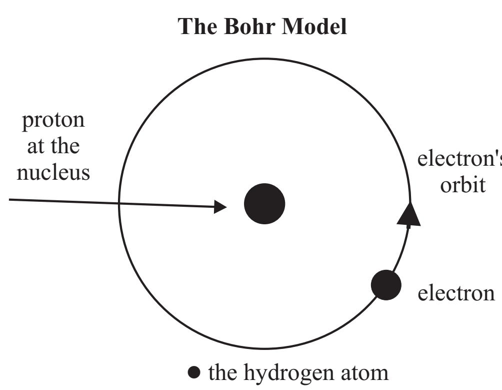
- The inadequacy of classical mechanics led to the development of *Quantum Mechanics*.

(*i*) The Hydrogen Atom and the Bohr Model

As the first example of the failure of classical physics to account for observed phenomena, we consider the case of the hydrogen atom. Rutherford model failed to explain two main observational features of the hydrogen atom:

(*a*) its stability and (*b*) the spectrum of its radiation. Let us consider these one at a time.

(*a*) An electron in a curved orbit is accelerated and hence must radiate. As it radiates its energy away, the radius of its orbit must decrease until eventually it collapses into the nucleus. Thus, the atom cannot be stable. But most of the atoms are stable.



Bohr's model of the hydrogen atom.

(*b*) The second discrepancy involves the observed radiation spectrum. The frequency of the radiated energy should be the same as the orbiting frequency. As the electron orbit collapses, its orbiting frequency increases continuously. We might thus expect the spectrum of radiation emitted by excited hydrogen atoms to be continuous. In contrast, the experimentally observed spectrum consists of families of discrete lines.

Bohr provided an explanation for both the spectral discreteness and the observed stability. He proposed that in solving for the orbital motion of the electron in its hydrogenic orbit one should impose an added condition:

The angular momentum of the electron must be equal to some integer multiple of $\hbar$.

$$l = n\hbar \ (n = 1, 2, 3...)$$

The quantisation implies that the laws of classical mechanics and of classical electro-magnetism are inapplicable at the atomic level.

(*ii*) Black Body Radiation

The observed variation of the spectral intensity $I(\nu)$ (power per unit area per unit frequency) of blackbody radiation as a function of frequency ν is shown in Fig. 2.1. From the curves we note that

(*i*) The intensity reaches a maximum at some frequency ν_m.

(*ii*) The frequency ν_m, as well as the height of the peak, increase with temperature.

The application of statistical thermodynamics and the ordinary laws of mechanics and electromagnetic theory led to the Rayleigh-Jeans formula

$$I(v) = \frac{8\pi v^2 kT}{c^3}.$$

This law, except for very low frequencies, is in total disagreement with experimental results. The law predicts an infinite amount of radiated intensity. Actually, the total radiated intensity is finite.

Max Planck resolved this controversy by postulating that the exchange of energy between atoms and radiation involves *discrete* amounts of energy. At a given frequency ν, the smallest amount of energy that can be exchanged is equal to

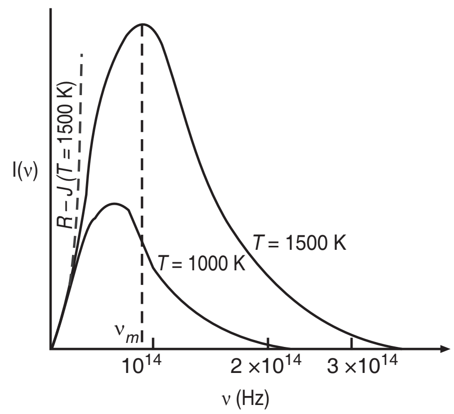


Fig. 2.1

$$E = h\nu.$$

Only multiples of $h\nu$ are involved in the interaction.

Applying this postulate to the problem of black body radiation theory, Planck obtained

$$I(\nu) = \frac{8\pi \nu^2}{c^3} \frac{h\nu}{e^{h\nu/kT} - 1}.$$

Planck's formula agrees with experimental curves. *The notion that field energy is quantized rather than a continuous quantity was a new and profound addition to physics*.

(*iii*) The Photoelectric Effect

A direct confirmation of the energy quantization of electromagnetic fields was provided by the phenomenon of photoelectric emission. When light of frequency ν is incident on a metal, electrons are emitted from the metallic surface only when $h\nu > \phi$. When $h\nu > \phi$, the electrons are emitted with a kinetic energy T, where

$$h\nu = \phi + T.$$

The energy of the photo-electron is independent of the intensity of light. The intensity of light determines merely the number (per second) of the emitted electrons. The explanation was provided by Einstein and invoked the electromagnetic field particles, photons, each carrying an energy $h\nu$. Electrons in the material are held back from the vacuum by an energy barrier of height ϕ. The impinging photon can transmit its energy $h\nu$ to an electron near the surface. If $h\nu < \phi$, this energy is insufficient to surmount the barrier and no electrons are ejected. If $h\nu > \phi$, the excess $T = h\nu - \phi$ is the kinetic energy of the electron leaving the surface.

(*iv*) The Compton Effect

The scattering of monochromatic X-rays from targets composed of light elements was studied by *Compton.* He found that the scattered radiation consists of two lines, one of the same wavelength as the incident radiation and one of slightly longer wavelength. The change in wavelength depended on the scattering angle. Compton was able to explain the measured angular dependence of wavelength shift perfectly when he assumed that individual photons of energy $E = h\nu$ and momentum $p = \frac{h\nu}{c}$ collided with individual electrons in such a way that momentum and energy were conserved. Compton's formula

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

gives the wavelength of the scattered photon in terms of incident wavelength and the angle at which the scattered photon is detected. This equation was verified by Compton experimentally.

The quantity $\frac{h}{m_0 c}$ in Compton's formula has dimensions of length and is called the Compton wavelength of the electron. Its magnitude is 2.43×10^{-12} m. This constant, which is characteristic of the X-ray scattering with wavelength shift, could not be reproduced by applying Maxwell's theory of electromagnetism to the scattering process.

(*v*) The Heat Capacity of Solids

Another experimental observation that could not be explained by ordinary physics was that of the heat capacity of solids. Classical equipartition of energy led to the prediction that the specific heat per kilo mole of solid elements should be $3R$. Dulong and Petit verified this result for many elements at high temperatures. However, the prediction failed completely in the low-termperature domain.

This disagreement between theory and experiment was resolved by Einstein and Debye who applied the Planck quantization condition

$$E = h\nu$$

to the mechanical oscillations of the lattice. The most profound effect of applying Planck's postulate to an oscillator is that its average thermal equilibrium excitation energy is no longer equal to kT (the classical value) but to

$$E = \frac{h\nu}{e^{h\nu/kT} - 1} \qquad ...(1)$$

Note that $E \to kT$ for $kT >> h\nu$. The application of Eq. (1) to the heat capacity problem resulted in excellent agreement with experiment.

the ejection of one or more secondary electrons from the surface. Suppose that a photoelectron striking dynode 1 produces x electrons by secondary emission. These electrons are then directed towards dynode 2 by making its potential higher than that of dynode 1. Suppose x electrons are again ejected by secondary emission for each incident electron. Then, for each electron emitted by the photosensitive plate, there are now x^2 electrons and so on. If there are several dynodes, each at a potential higher than the preceding one, an avalanche of electrons reaches the collector plate A. A strong current then flows in the outer circuit. This device is used to amplify very weak light signals.

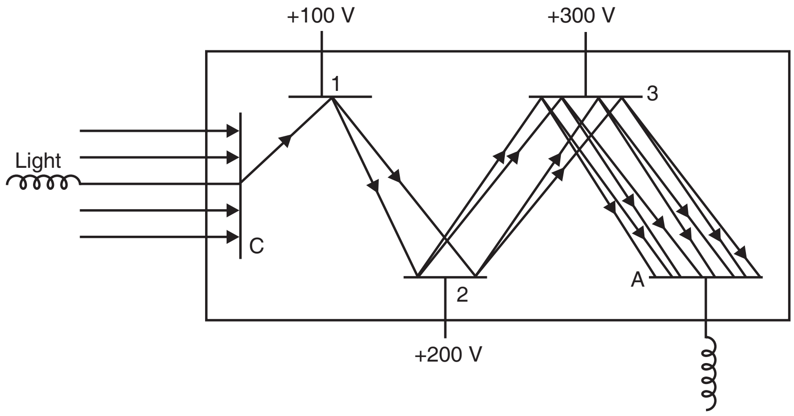


Fig. 2.2

(***iii***) Photoelectric cells are used to compare the illuminating powers of two light sources. They are also used in the measurement of the intensity of illumination of a light source.

(***iv***) **Sound reproduction in films.** The film is provided with a sound track at one edge. Light passing through the sound track of the film falls on a photocell. Current is produced, which fluctuates correspondingly with the intensity of sound recorded in the sound track. The current impulses are converted to sound by speakers.

(***v***) **Automatic operation of street lights.** A photoelectric cell, located in a street light circuit, switches off the street light when sunlight is incident on the cell. When sunlight fades and it becomes dark, the photoelectric cell switches on the street lights.

2.3 PLANCK'S QUANTUM THEORY

The distribution of energy in the spectrum of a black body. If the radiation emitted by a black body at a fixed temperature is analysed by means of a suitable spectroscopic arrangement, it is found to spread up into a continuous spectrum. The total energy is not distributed uniformly over the entire range of the spectrum.

Experimental arrangement. The distribution of energy in various parts of the spectrum was experimentally studied by Lummer and Pringsheim. The radiation from the black body was rendered into a parallel beam by the concave mirror [Fig. 2.3]. It is then allowed to fall on a prism of fluorspar to resolve it into a spectrum. The spectrum is brought to focus by another concave mirror on to a linear bolometer. The bolometer is connected to a galvanometer. The deflections in the galvanometer corresponding to different λ are noted by rotating the prism table. Then curves are plotted for E_λ versus λ. The experiment is done with the black body at different temperatures. The curves obtained are shown in Fig. 2.4.

Results. (*i*) At any given temperature, E_λ first increases with λ, reaching a maximum value corresponding to a particular wavelength λ_m and then decreases for longer wavelengths.

(*ii*) The value of E_λ for any λ increases as temperature increases.

(*iii*) The wavelength corresponding to the maximum energy shifts to shorter wavelength side as the temperature increases. This confirms Wien's displacement law $\lambda_m T$ = constant.

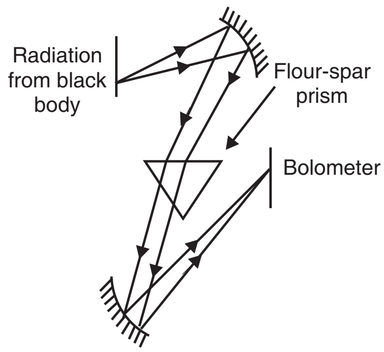


Fig. 2.3

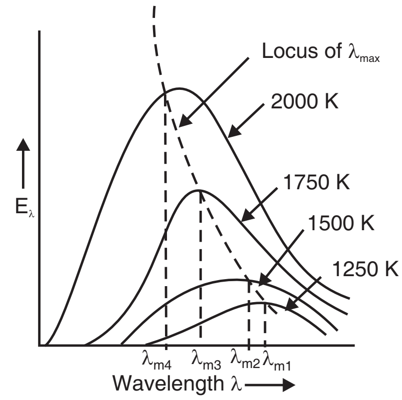


Fig. 2.4

(*iv*) Total energy emitted per unit area of the source per second at a given temperature is $\int_0^\infty E_\lambda \, d\lambda$. It will be represented by the total area between the curve for that temperature and the λ-axis. This area is found to be proportional to the fourth power of the absolute temperature. This verifies *Stefan's law*.

Wien's Displacement Law. *The wavelength of the most strongly emitted radiation in the continuous spectrum from a full radiator is inversely proportional to the absolute temperature of that body, i.e.,* $\lambda_m T = b$.

Here, b is Wien's constant 2.898×10^{-3} mK.

Planck's hypothesis. According to the classical theory of radiation, energy changes of radiators take place continuously. The classical theory failed to explain the experimentally observed distribution of energy in the spectrum of a black body. Planck succeeded in deriving a formula which agrees extremely well with experimental results. He discarded both the idea of radiation being a continuous stream as well as the law of equipartition of energy. He suggested the *quantum theory of radiation*. His assumptions are:

(1) A black-body radiation chamber is filled up not only with radiation, but also with *simple harmonic oscillators* or *resonators* of molecular dimensions. They can vibrate with all possible frequencies.

(2) The oscillators or resonators cannot radiate or absorb energy continuously. But an oscillator of frequency ν can only radiate or absorb energy in units or quanta of magnitude $h\nu$. h is a universal constant called Planck's constant. The emission of radiation corresponds to a decrease and absorption to an increase in the energy and amplitude of an oscillator.

Derivation of Planck's law of radiation. Let N be the total number of Planck's resonators and E their total energy. Then, average energy per oscillator $= \bar{\varepsilon} = E/N$.

$$N = N_0 + N_0 e^{-\varepsilon/kT} + N_0 e^{-2\varepsilon/kT} + \cdots + N_0 e^{-r\varepsilon/kT} + \cdots$$

Here N_0 = number of resonators having 0 energy.

$N_0 e^{-\varepsilon/kT}$ = number of resonators having energy ε,

$N_0 e^{-2\varepsilon/kT}$ = number of resonators having energy 2ε,

$N_0 e^{-r\varepsilon/kT}$ = number of resonators having energy $r\varepsilon$ and so on.

Putting $\varepsilon/kT = x,$

$$N = N_0 + N_0 e^{-x} + N_0 e^{-2x} + \cdots\cdots\cdots N_0 e^{-rx}$$

$$\therefore \quad N = \frac{N_0}{1-e^{-x}} \qquad ...(1)$$

The total energy of Planck's resonators is

$$E = 0 \times N_0 + \varepsilon \times N_0 e^{-x} + 2\varepsilon \times N_0 e^{-2x} + \cdots + r\varepsilon \times N_0 e^{-rx} + \cdots\cdot$$

$$Ee^{-x} = \varepsilon N_0 e^{-2x} + 2\varepsilon N_0 e^{-3x} + \cdots + r\varepsilon N_0 e^{-(r+1)x}$$

Subtracting, $E(1 - e^{-x}) = \varepsilon N_0 e^{-x} + \varepsilon N_0 e^{-2x} + \varepsilon N_0 e^{-3x} + \cdots$

$$= \frac{\varepsilon N_0 e^{-x}}{1-e^{-x}}$$

$$\therefore \quad E = \frac{\varepsilon N_0 e^{-x}}{(1-e^{-x})^2} \qquad ...(2)$$

Average energy of a resonator $= \bar{\varepsilon} = \dfrac{E}{N} = \dfrac{\varepsilon e^{-x}}{1-e^{-x}} = \dfrac{\varepsilon}{e^x - 1}$

According to Planck's hypothesis, $\varepsilon = h\nu$. Further $\nu = c/\lambda$.

Hence,

$$\varepsilon = \frac{hc}{\lambda} \quad \text{and} \quad x = \frac{\varepsilon}{kT} = \frac{hc}{\lambda kT}$$

$$\therefore \quad \bar{\varepsilon} = \frac{hc/\lambda}{\left(e^{hc/\lambda kT} - 1\right)} \qquad ...(3)$$

Number of oscillators per unit volume in the wavelength range λ and $\lambda + d\lambda = 8\pi\lambda^{-4}\,d\lambda$. ...(4)

Hence, energy density of radiation between wavelengths λ and $\lambda + d\lambda$ = (average energy of a Planck's oscillator) × (number of oscillators per unit volume).

$$E_\lambda\, d\lambda = \frac{hc/\lambda}{\left(e^{hc/\lambda kT} - 1\right)} \times 8\pi\lambda^{-4}\, d\lambda$$

$$E_\lambda\, d\lambda = \frac{8\pi hc\lambda^{-5}}{\left(e^{hc/\lambda kT} - 1\right)} d\lambda \qquad ...(5)$$

or

$$E_\nu d\nu = \frac{8\pi h\nu^3}{c^3\left(e^{h\nu/kT} - 1\right)} d\nu \qquad ...(6)$$

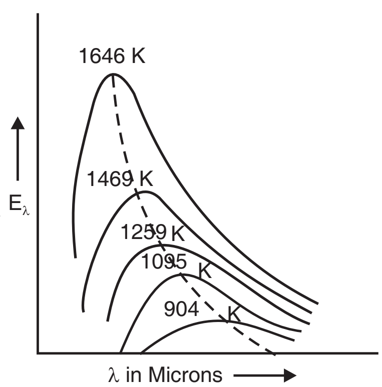


Fig. 2.5

Here $E_\nu\, d\nu$ is the energy density belonging to the range $d\nu$. Eq. (5) represents Planck's radiation law in terms of wavelength. Planck's formula fits the experimental curve very closely [Fig. 2.5].

- Planck's formula reduces to Wien's formula for small wavelengths. When λ is small, $e^{hc/\lambda kT}$ is large when compared to 1. Hence Eq. (5) reduces to

$$E_\lambda d\lambda = 8\pi\, h\, c\, \lambda^{-5}\, e^{-hc/\lambda kT} d\lambda \qquad ...(7)$$

This is *Wien's law*.

- Planck's formula reduces to Rayleigh Jean's formula for longer wavelengths.

  When λ is large, $e^{hc/\lambda kT} \approx 1 + (hc/\lambda kT)$.

  Hence Planck's law reduces to

$$E_\lambda \, d\lambda \;=\; 8\pi \frac{hc\lambda^{-5}}{(hc/\lambda kT)} d\lambda = 8\pi kT\lambda^{-4}\, d\lambda \qquad ...(8)$$

  This is *Rayleigh-Jeans formula*.

2.4 Photo Electric Effect

Whenever light or electromagnetic radiations (such as X-rays, Ultraviolet rays) fall on a metal surface, it emits electrons. *This process of emission of electrons from a metal plate, when illuminated by light of suitable wavelength*, *is called the photoelectric effect.* The electrons emitted are called the *photoelectrons*. In the case of alkali metals, photoelectric emission occurs even under the action of visible light. Zinc, cadmium etc., are sensitive to only ultraviolet light.

The Nature of Photo-particles

Experimental arrangement. The apparatus consists of two plates A and C placed in an evacuated quartz bulb (Fig. 2.6).

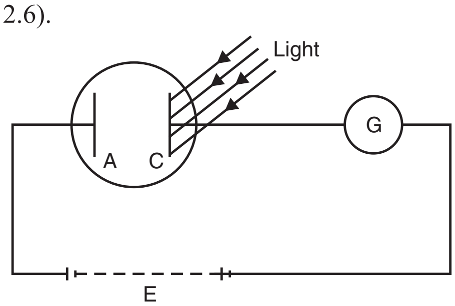


Fig. 2.6

The galvanometer (G) and battery (E) are connected as shown. When ultraviolet light is incident on the negative plate C, a current flows in the circuit as indicated by the galvanometer. But when light falls on the positive plate A, there is no current in the circuit. These observations show that photo-particle must be negatively charged.

2.5 EXPERIMENTAL INVESTIGATIONS ON THE PHOTOELECTRIC EFFECT

Apparatus: Photoelectric effect can be studied in detail with the help of the apparatus shown in Fig. 2.7.

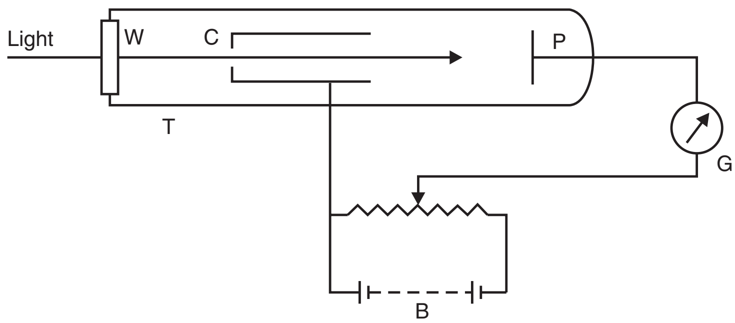


Fig. 2.7

It consists of an evacuated glass tube *T* with a quartz window *W*. *P* is a photoelectrically sensitive plate. *C* is a hollow cylinder and it has a small hole that permits the incident light to fall on the plate *P*. *P* is connected to the negative end. *C* is connected to the positive terminal of a battery *B*.

Working. When light from some source falls on the plate *P*, the photoelectrons are ejected out of the plate *P*. These photoelectrons are attracted by the positively charged cylinder *C*. Hence a photoelectric current flows from *P* to *C* in the bulb and from *C* to *P* outside the bulb. This current can be measured from the deflection produced in the galvanometer *G*. It is found that the strength of the photoelectric current increases as the potential of *C* is more and more positive with respect to *P*. The deflection in *G* decreases when the potential of *C* is negative with respect to *P*. The results obtained are summarised into four statements. They are called the laws of photoelectric emission.

Laws of photoelectric emission. (*i*) *For every metal, there is a particular minimum frequency of the incident light, below which there is no photoelectric emission, whatever be the intensity of the radiation. This minimum frequency, which can cause photoelectric emission, is called the threshold frequency.*

(*ii*) *The strength of the photoelectric current is directly proportional to the intensity of the incident light, provided the frequency is greater than the threshold frequency.*

(*iii*) *The velocity and hence the energy of the emitted photoelectrons is independent of the intensity of light and depends only on the frequency of the incident light and the nature of the metal.*

(*iv*) *Photoelectric emission is an instantaneous process. The time lag, if any, between incidence of radiation and emission of the electrons, is never more than* 3×10^{-9} *sec.*

Failure of the electromagnetic theory. The above experimental facts could not be explained on the basis of the electromagnetic theory of light.

(1) Calculations showed that it would require about 500 days to dislodge a photoelectron from sodium by exposure to violet light of wavelength 4000 Å. Experimentally, however, we observe that electron ejection commences without delay.

(2) According to the classical theory, light of greater intensity should impart greater K.E. to the liberated electrons. But, this does not happen. Also, the velocity of the emitted electron should not depend on the frequency of the incident light. But it does.

The phenomenon was adequately explained by Einstein on the basis of Planck's Quantum theory of radiation.

Quantum theory. According to Planck, the energy of a monochromatic wave with frequency ν can only assume those values which are integral multiples of energy $h\nu$. *i.e.*, $E_n = nh\nu$, where n is an integer referring to the number of "*Photons*". Thus the energy of a single *PHOTON* of frequency ν is $E = h\nu$.

2.6 EINSTEIN'S PHOTOELECTRIC EQUATION

According to Einstein, light of frequency ν consists of a shower of corpuscles or photons each of energy $h\nu$. When a photon of light of frequency ν is incident on a metal, the energy is completely transferred to a free electron in the metal. A part of the energy acquired by the electron is used to pull out the electron from the surface of the metal and the rest of it is utilised in imparting K.E. to the emitted electron. Let ϕ be the energy spent in extracting the electron from the emitter to which it is bound (photoelectric work function) and $\frac{1}{2} mv^2$ the K.E. of the photoelectron.

Then $$h\nu = \phi + \frac{1}{2} mv^2 \qquad ...(1)$$

This relation is called the *Einstein's Photoelectric equation.* If ν_o is the threshold frequency which just ejects an electron from the metal without any velocity then, $\phi = h\nu_o$.

$$\therefore \quad h\nu = h\nu_o + \frac{1}{2} mv_{max}^2 \qquad ...(2)$$

Here, v_{max} is the maximum velocity acquired by the electron.

or $$\frac{1}{2} mv^2_{max} = h(\nu - \nu_0) \qquad ...(3)$$

- *The work function of a metal is defined as the energy which is just sufficient to liberate electrons from the metal surface with zero velocity.*
- Equation (3) suggests that the energy of the emitted photoelectrons is independent of the intensity of the incident radiation but increases with the frequency.

Experimental verification of Einstein's Photoelectric Equation—Millikan's Experiment.

Theory. Millikan's experiment is based on the "*stopping potential*". The stopping potential is the necessary retarding potential difference required in order to just halt the most energetic photoelectron emitted.

The K.E. of a photoelectron leaving the surface of a metal irradiated with light of frequency ν $\Big\} = \frac{1}{2} mv_{max}^2 = h\nu - \phi.$

Let V be the P.D. which is applied between the emitter and a collecting electrode in order to prevent the photoelectron from just leaving the emitter, the emitter being maintained at a positive potential with respect to the collector. Then,

$$eV = \frac{1}{2} mv_{max}^2$$

$$\therefore \quad eV = h\nu - \phi$$

or $$V = \frac{h}{e}\nu - \frac{\phi}{e} \qquad ...(1)$$

ϕ is constant for a given metal; h and e are also constants.

Hence, Eq. (1) represents a straight line. V is measured for different values of ν. A graph is then plotted between the stopping potential (V) taken along the Y-axis and the frequency of light (ν) taken along the X-axis. The graph is a straight line (Fig. 2.8). The slope of the straight line

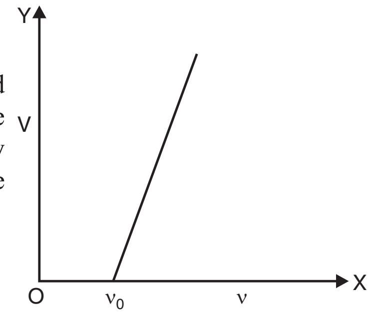


Fig. 2.8

$$\tan\theta = \frac{h}{e}$$

$$\therefore \qquad h = e\tan\theta \qquad ...(2)$$

Hence the value of h (Planck's constant) can be calculated. The intercept on the X-axis gives the threshold frequency ν_o for the given emitter. From this, photoelectric work function = $\phi = h\ \nu_o$ is calculated.

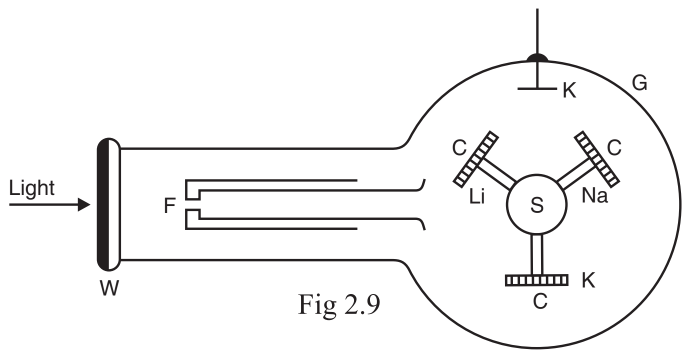


Fig 2.9

Experiment. Millikan's apparatus is shown in Fig. 2.9. Alkali metals are employed as emitters, since they readily exhibit photoelectric emission even with visible light. Cylindrical blocks (C) of sodium, potassium or lithium are mounted on a spindle S at the centre of the glass flask G. The flask is evacuated to a very high vacuum to free the metals from all absorbed gases and to prevent their oxidation. The spindle can be rotated from outside by an electromagnet. As each metal block passes by the adjustable sharp edge K, a thin layer of it is removed, thus exposing a fresh surface of the metal to the irradiating light entering the flask through a quartz window W. Monochromatic light provided by a spectroscope is used to illuminate the fresh metal surfaces. The photoelectrons are collected by a Faraday cylinder F. The Faraday cylinder is made of copper oxide which is not photosensitive. The photocurrent is measured by an electrometer connected to the Faraday cylinder.

The stopping potential of the liberated photoelectrons is measured by raising the emitter surface to a positive potential, just sufficient to prevent any of the electrons from reaching the collector (F). The stopping potential is the positive potential applied to the emitter, which corresponds to zero current in the electrometer. The stopping potential (V) is determined for different wavelengths of the incident light. The value of V should be corrected for any contact potential between the metal (C) and Faraday cylinder (F). On plotting V against ν, we get a straight line. Measuring the slope of the

straight line, the value of h/e is obtained. Then substituting the known value of e, h is calculated. The value of h calculated in this way agrees fairly well with the value obtained by other methods. Thus the Einstein's equation can be verified experimentally.

EXERCISE

1. The velocity of photoelectron depends upon the .... of the incident photon only.

[**Ans.** Frequency]

2. .... is known as the Einstein's photoelectric equation.

[**Ans.** $h\nu = \phi + 1/2\, mv^2$]

3. At threshold frequency, the kinetic energy of emitted photoelectron is ....

[**Ans.** zero](*B.U., April 2013*)

4. The photoelectric work function ϕ = ... [**Ans.** $\phi = h\nu_o$]

5. Millikan's experiment is based on ....

(*a*) developing potential (*b*) high potential (*c*) stopping potential (*d*) negative potential.

[**Ans.** (*c*)]

6. In photoconductive cell, as the intensity of radiation increases, ... of semiconductor mterial decreases.

(*a*) elasticity (*b*) hardness (*c*) resistance (*d*) none of these

[**Ans.** (*c*)]

7. Explain the Richardson and Compton experiment to study the photoelectric phenomena.

8. State and explain laws of photoelectric emission.

9. Derive Einstein's photoelectric equation.

10. Calculate the work function of sodium, in electron-volts, given that the threshold wavelength is 6800 Å, and $h = 6.625 \times 10^{-34}$ Js.

[**Sol.** $\phi = h\nu_0 = hc/\lambda_0$

Here, $h = 6.625 \times 10^{-34}$ Js; $c = 3 \times 10^8$ ms^{-1} and $\lambda_0 = 6800 \times 10^{-10}$ m.

$$\therefore \quad \phi = \frac{(6.625\times10^{-34})(3\times10^{8})}{(6800\times10^{-10})}\text{ J} = \frac{(6.625\times10^{-34})(3\times10^{8})}{(6800\times10^{-10})(1.6\times10^{-19})}\text{ eV}$$

$= 1.827$ eV.]

11. The photoelectric threshold for a metal is 3000 Å. Find the kinetic energy of an electron ejected from it by radiation of wavelength 1200 Å.

[**Sol.** K.E. of the electron $= \frac{1}{2}mv^2 = h(v - \nu_0)$

$$= \frac{hc(\lambda_0 - \lambda)}{\lambda\,\lambda_0} = \frac{(6.62\times10^{-34})(3\times10^{8})(1800\times10^{-10})}{(3000\times10^{-10})(1200\times10^{-10})} = 9.93 \times 10^{-19}\text{ J} = 6.2\text{ eV}]$$

12. Discuss the relation between photoelectric current and retarding potential in photoelectric effect.

13. With necessary theory, discuss the Millikan's experimental verification of Einstein's photoelectric equation.

14. Discuss the distribution of energy in the spectrum of a black body and its results.

15. Derive an expression for Planck's law of radiation.

UNIT III

CONCEPT OF MATTER WAVES

de Broglie's concept of matter waves – expression for de Broglie's wavelength – phase velocity – group velocity relationship. Heisenberg's Uncertainty Principle – Elementary proof of Heisenberg's uncertainty relations.

3.1 MATTER WAVES

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

$$\lambda = \frac{h}{p} = \frac{h}{mv}, \qquad ...(1)$$

Here, 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 ν has the momentum

$$p = h\nu/c.$$

But $\nu = c/\lambda$. 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

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

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

$$\lambda = h/mv.$$

3.1.1. Expression for de Broglie Wavelength

De Broglie derived an expression for the wavelength of matter waves on the analogy of radiation.

Based on Planck's theory of radiation, the energy of a photon (quantum) is

$$E = h\nu = \frac{hc}{\lambda} \qquad ...(1)$$

Here, c is the vacuum velocity of light and λ its wavelength.

According to Einstein mass-energy relation,

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

From Eqs. (1) and (2),

$$mc^2 = \frac{hc}{\lambda}$$

or

$$\lambda = \frac{h}{mc} = \frac{h}{p} = \frac{h}{\text{momentum}} \qquad ...(3)$$

Here, $mc = p$ is the momentum associated with photon.

De Broglie suggested that this equation for wavelength is a perfectly general one, applying to material particles as well as to photons. In the case of particles,

$$\text{momentum} = mv.$$

Hence the de Broglie wavelength of a particle is

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

3.1.2. Other Expressions for de-Broglie Wavelength

(*i*) **For a Free particle:** If E_k is the kinetic energy of the material particle, then

$$p = \sqrt{(2mE_k)}$$

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

$$\lambda = \frac{h}{\sqrt{2mE_k}} \qquad ...(1)$$

(*ii*) **For a charged particle accelerated through a potential difference *V*:** If a charged particle carrying charge q is accelerated through a potential difference V volts, then kinetic energy $E_k = qV$.

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

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

(*iii*) **For thermal neutrons:** Kinetic energy of thermal neutrons is $E_k = kT$.

Here, k = Boltzmann constant,

T = temperature at which neutrons are enclosed in the chamber.

Therefore, the de-Broglie wavelength of a material particle at temperature T is

$$\lambda = \frac{h}{\sqrt{(2mE_k)}} = \frac{h}{\sqrt{2mkT}} \qquad ...(3)$$

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 $v << c$, we can take $m = m_0 \rightarrow$ the rest mass. Hence

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

$$= \mathbf{4.0 \times 10^{-34}\ m.}$$

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 $v << c$, so $m = m_0 = 9.1 \times 10^{-31}$ kg.

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

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

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

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

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

$$= \frac{1.227 \times 10^{-9}\,\text{m}}{\sqrt{V}} = \frac{1.227}{\sqrt{V}}\,\mathbf{nm}$$

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 GeV.

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

The total energy of the proton is

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

The kinetic energy of the proton is

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

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*

$$\lambda = \frac{h}{\sqrt{2 m_0 qV\left(1 + \dfrac{qV}{2 m_0 c^2}\right)}}$$

Sol. We use the relativistic formula to find momentum.

Kinetic energy $E_k = qV$.

$$E^2 = p^2c^2 + m_0^2 c^4,\ E = E_k + m_0 c^2 = qV + m_0 c^2$$

So, $$p^2c^2 = E^2 - m_0^2 c^4 = (qV + m_0 c^2)^2 - m_0^2 c^4 = q^2 V^2 + 2 m_0 c^2 qV$$

$$p^2 = 2m_0 qV\left(1 + \frac{qV}{2m_0 c^2}\right) \text{ or } p = \sqrt{2m_0 qV\left(1 + \frac{qV}{2 m_0 c^2}\right)}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2 m_0 qV\left(1 + \dfrac{qV}{2 m_0 c^2}\right)}}$$

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.

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

$$= \frac{1.227}{\sqrt{V}} \times \frac{1}{\sqrt{1 + 9.768 \times 10^{-7} V}}\ \text{nm}$$

3.1.3. Phase velocity (or Wave Velocity) of de Broglie Waves

The phase velocity v_p of a monochromatic wave is the velocity with which a definite phase of the wave, such as its crest or trough, is propagated in a medium.

The equation of motion of a plane wave of frequency ν and wavelength λ moving in the x-direction is

$$y = A \cos(\omega t - kx).$$

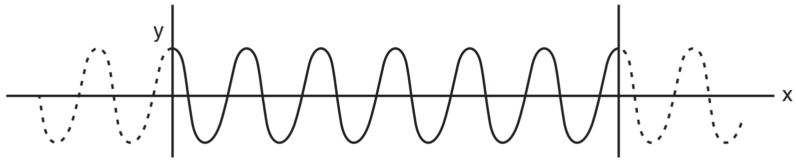


Fig. 3.1

Here, A is the amplitude of the wave (Fig. 3.1).

ω (= $2\pi\nu$) is the angular frequency and k (= $2\pi/\lambda$) is the propagation constant.

This wave moves with a phase velocity

$$v_p = \nu\lambda = \omega/k$$

- 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 ν be the frequency of the associated wave. We equate the quantum expression $E = h\nu$ with the relativistic formula for total energy $E = mc^2$. So we get

$$h\nu = mc^2 \text{ or } \nu = mc^2/h.$$

Let v_p be the de Broglie wave velocity. Then,

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

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

3.1.4. Group Velocity

It is possible to form a concentrated *wave packet* by taking a sum of a large number of plane waves with slightly different wavelengths and frequencies. When such a group travels in a dispersive medium, the phase velocities of its different components are different. The observed velocity is, however, the velocity with which the maximum amplitude of the group advances in the medium. This is called the "group velocity". Thus, *the group velocity is the velocity with which the energy in the group is transmitted*. The individual waves travel "inside" the group with their phase velocities.

- *The velocity with which the centre of a wave group i.e., maximum amplitude, moves is called the group velocity of the wave group.*

3.1.5. 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 superpostition 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.

$$y = y_1 + y_2$$

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

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

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

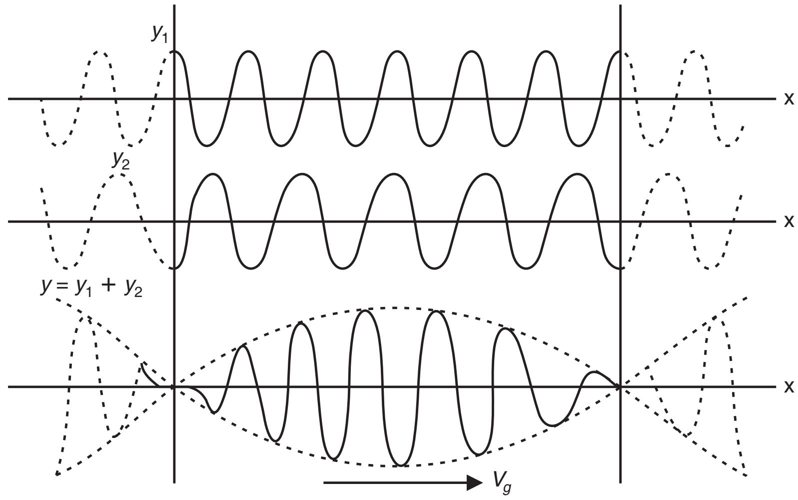


Fig. 3.2

$$2\omega + \Delta\omega \approx 2\omega$$

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

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

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 ω and wave number k that has superimposed upon it a modulation of angular frequency $\frac{1}{2}\Delta\omega$ (Fig. 3.2).

The velocity v_g of the wave groups is

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

When ω and k have continuous spreads, the group velocity is given by

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

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

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

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

By differentiation, we obtain

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

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

The group velocity v_g of the de Broglie 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 (v_g) and Wave Velocity or Phase Velocity (v_p)

We have the relations,

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

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

The wave number is given by

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

$$\therefore \quad \frac{dk}{d\lambda} = -\frac{2\pi}{\lambda^2} \quad ...(3)$$

Also
$$\omega = 2\pi\nu = 2\pi\frac{v_p}{\lambda}$$

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

or
$$\frac{d\omega}{d\lambda} = -\frac{2\pi}{\lambda^2}\left[v_p-\lambda\frac{dv_p}{d\lambda}\right] \quad ...(4)$$

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

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

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

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

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).

$$\therefore \quad v_g < v_p.$$

This is the case with de Broglie waves.

(ii) *For non-dispersive medium*

$$v_p \neq f(\lambda). \ \frac{dv_p}{d\lambda} = 0. \ \therefore v_g = v_p$$

This result is true for electromagnetic waves in vacuum.

- If the phase velocity is the same for all wavelengths, as is true for light waves in empty space, the group and phase velocities are the same.

3.2 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.

Example 1. According to this principle, the position and momentum 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:

$$\Delta x \ \Delta p \geq \hbar/2.$$

The product of the two errors is approximately of the order of Planck's constant $\hbar$.

- If Δx is small, Δp will be large and vice versa.

If one quantity is measured accurately, the other quantity becomes

Example 2. Consider the wave group of Fig. 7.15.

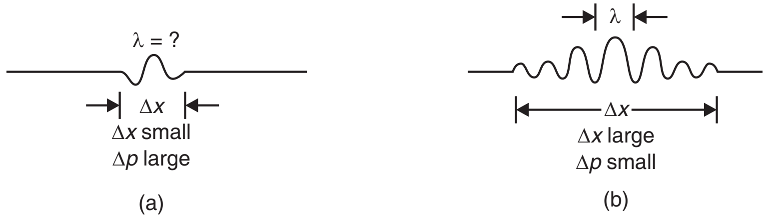


Fig. 3.3

(*a*) *A narrow de Broglie wave group*. The narrower its wave group, the more precisely a particle's position can be specified (Fig. 3.3*a*).

But, the wavelength of the waves in a narrow packet is not well defined because there are not enough waves to measure λ accurately. Since $\lambda = \frac{h}{mv}$, the particle's momentum *mv* is not a precise quantity. If we make a series of momentum measurements, we will find a broad range of values.

(*b*) *A wide wave group*. Now the wavelength λ can be precisely determined (Fig. 3.3*b*). The momentum *mv* is therefore a precise quantity. But the position of the particle is not well defined.

- *It is impossible to know both the exact position and exact momentum of an object at the same time.*

Illustration (i) : Determination of position with γ-ray microscope.

Suppose we try to measure the position and linear momentum of an electron using an imaginary microscope with a very high resolving power (Fig. 3.4).

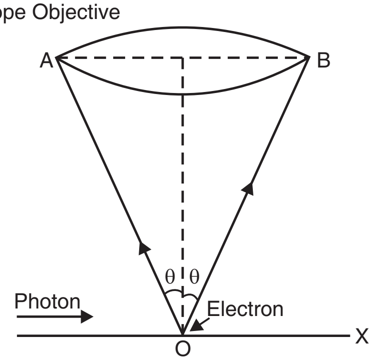


Fig. 3.4

Uncertainty in position measurement

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

$$\Delta x = \frac{\lambda}{2 \sin \theta} \qquad ...(1)$$

Here, Δ*x* 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.

Uncertainty in momentum measurement

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 2θ. 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 $OA = -\dfrac{h}{\lambda}\sin\theta$

The component of this momentum along $OB = \dfrac{h}{\lambda}\sin\theta$.

The uncertainty in the momentum measurement in the x-direction is

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

$$\therefore \qquad \Delta x \times \Delta p_x = \frac{\lambda}{2\sin\theta} \times \frac{2h}{\lambda}\sin\theta = h.$$

A more sophisticated approach will show that $\Delta x\, \Delta p_x \geq \hbar/2$.

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

A beam of electrons is transmitted through a slit and received on a photographic plate P kept at some distance from the slit (Fig. 3.5).

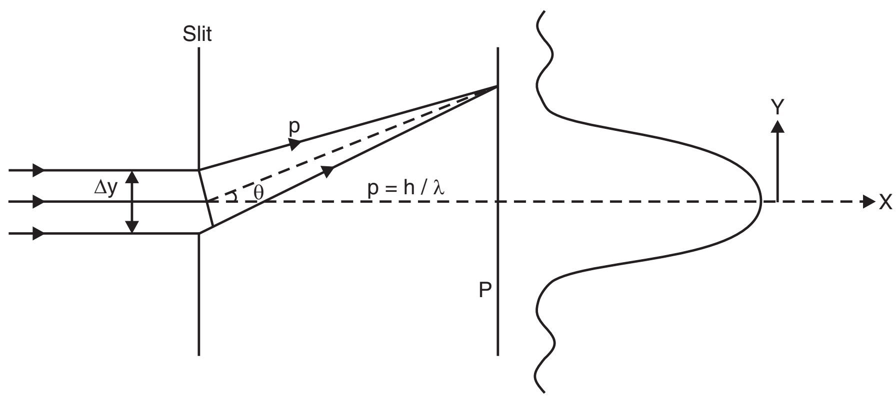


Fig. 3.5

- **Uncertainty in position measurement**

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).

λ is the wavelength of the electrons. θ is the angle of deviation corresponding to first minimum.

From the theory of diffraction in optics,

$$\Delta y = \frac{\lambda}{\sin\theta}. \qquad ...(1)$$

This is the uncertainty in determining the position of electron along y-axis.

- **Uncertainty in momentum measurement**

Initially the electrons are moving along X-axis. 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.

p is the momentum of the electron on emerging from the slit.

The component of momentum of electron along y-axis is $p \sin \theta$.

The electron may be anywhere within the pattern from angle $-\theta$ to $+\theta$. So, 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

$$\Delta p_y = 2p \sin \theta = \frac{2h}{\lambda} \sin \theta \qquad \left(\because \lambda = \frac{h}{p} \right) \qquad ...(2)$$

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

i.e., $\Delta y \, \Delta p_y \geq \frac{\hbar}{2}$, which is Heisenberg's uncertainty principle.

3.2.1. Energy-Time Uncertainty Relation

Consider a free particle of mass m moving with velocity v.

Its kinetic energy is

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

Here, $p = mv$ = momentum of particle.

Uncertainty in energy is given by

$$\Delta E = \frac{2p \, \Delta p}{2m} = \frac{p \, \Delta p}{m} = \frac{mv \, \Delta p}{m} = v \, \Delta p.$$

But
$$v = \frac{\Delta x}{\Delta t}$$

$$\therefore \qquad \Delta E = \frac{\Delta x}{\Delta t} \Delta p$$

$$\Delta E \, \Delta t = \Delta x \, \Delta p$$

Uncertainty relation in terms of position and momentum is

$$\Delta x \, \Delta p \geq \hbar/2$$

$$\therefore \qquad \Delta E \, \Delta t \geq \frac{\hbar}{2}.$$

3.2.2. Applications of Uncertainty Principle

- **Non-existence of Electron in the Nucleus**

Example 1. *Prove the nonexistence of electron in the nucleus on the basis of uncertainty principle.*

Sol. Nuclear diameter is of the order of 10^{-15} m. For an electron to exist inside a nucleus, the uncertainty in its position must be at least of this order. That is, $\Delta x \simeq 10^{-15}$ m.

The uncertainty in the electron momentum is

$$\Delta p \cong \frac{\hbar}{2(\Delta x)} \cong \frac{1.055 \times 10^{-34}}{2 \times 10^{-15}} = 0.527 \times 10^{-19} \text{ kg ms}^{-1}$$

Energy of the electron, $E = (c^2 p^2 + m_0^2 c^4)^{1/2} \simeq cp$

$$E = (3 \times 10^8 \text{ ms}^{-1}) \times (0.527 \times 10^{-19} \text{ kg ms}^{-1}) = 1.581 \times 10^{-11} \text{ J}$$

$$E = \frac{1.581 \times 10^{-11}}{1.6 \times 10^{-19}} \text{ eV} = 98.8 \text{ MeV}$$

For an electron to be a constituent of the nucleus, it should have an energy of the order of 98.8 MeV. However, the energy of an electron emitted in a β-decay experiment is of the order of 3 MeV. Hence, we conclude that electrons do not reside in the nucleus.

- **Zero-Point Energy of a Harmonic Oscillator**

EXAMPLE 2. *Using the uncertainty principle, estimate the ground state energy of the harmonic oscillator.*

SOL. Assume that the particle position is uncertain by Δx. Then, from the uncertainty principle, the uncertainty in particle momentum is $\Delta p = \hbar/(2\Delta x)$.

Total energy of the linear harmonic oscillator is

$$E = \frac{1}{2}k(\Delta x)^2 + \frac{(\Delta p)^2}{2m} = \frac{1}{2}k(\Delta x)^2 + \frac{\hbar^2}{8m(\Delta x)^2} \qquad ...(1)$$

The value of E will be minimum when $\frac{dE}{d(\Delta x)} = 0$

$$k\Delta x - \frac{\hbar^2}{4m(\Delta x)^3} = 0 \text{ or } \Delta x = \left(\frac{\hbar^2}{4mk}\right)^{1/4}.$$

Substituting the value of Δx in Eq. (1), we get

$$E_{\min} = \frac{1}{2}k\left(\frac{\hbar^2}{4mk}\right)^{1/2} + \frac{\hbar^2}{8m}\left(\frac{4mk}{\hbar^2}\right)^{1/2} = \frac{\hbar}{2}\left(\frac{k}{m}\right)^{1/2} = \frac{\hbar\omega}{2}.$$

- **The Ground State Energy and the Radius of the Hydrogen Atom**

EXAMPLE 3. *Consider an electron of momentum p in the Coulomb field of a proton. The total energy is*

$$E = \frac{p^2}{2m} - \frac{e^2}{(4\pi\varepsilon_0)r},$$

where r is the distance of the electron from the proton. Assuming that the uncertainty Δr of the radial coordinate is $\Delta r \approx r$ and that $\Delta p \approx p$, use Heisenberg's uncertainty principle $\Delta r \Delta p = \hbar$ to obtain an estimate of the size and the energy of the hydrogen atom in the ground state.

SOL. From the uncertainty principle, $\Delta p \geq \frac{\hbar}{\Delta r} = \frac{\hbar}{r}$.

The momentum p cannot be less than the uncertainty Δp. Hence, the minimum possible momentum is

$$p = \frac{\hbar}{r} \qquad ...(1)$$

The total energy of the electron is given by

$$E = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r} \qquad ...(2)$$

$$\therefore \quad E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r} \qquad ...(3)$$

The system will be in the state of lowest energy at the value of r given by

$$\frac{dE}{dr} = 0$$

or $$-\frac{\hbar}{mr^3}+\frac{e}{4\pi\varepsilon_0 r^2} = 0$$

or $$r = \frac{(4\pi\varepsilon_0)\hbar^2}{me^2}$$

This is same as the expression obtained for the first Bohr radius a_0. Its value is

$$r = a_0 = 0.53 \text{ Å} \quad ...(4)$$

Substituting in Eq. (3), the ground state energy of the hydrogen atom is

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{me^2}{4\pi\varepsilon_0\hbar^2}\right)^2 - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{me^2}{4\pi\varepsilon_0\hbar^2}\right) = -\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2}$$

$$\therefore \quad E_0 = -13.6 \text{ eV} \quad ...(5)$$

- **Evidence for finite width of the spectral lines**

Example 4. *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.*

Sol. We have, $\Delta E\, \Delta t \geq \hbar/2$.

$$\therefore \quad \Delta E \geq \frac{\hbar}{2\Delta t} = \frac{1.054\times10^{-34}}{2(10^{-8})}$$

$$\therefore \quad \Delta E \geq 0.527 \times 10^{-26} \text{ J} = 3.29 \times 10^{-8} \text{ eV}.$$

This is known as the *energy width* of an excited state.

The width of the spectral line when the atom de-excites to the ground state is

$$\Delta\nu = \frac{\Delta E}{h}$$

$$= \frac{0.527\times10^{-26}}{6.63\times10^{-34}}$$

$$\Delta\nu = 8 \times 10^6 \text{ Hz}$$

This is the limit to the accuracy with which the frequency of the radiation emitted by an atom can be determined.

3.2.3. Mathematical Proof of Uncertainty Principle for One Dimensional Wave-packet

We shall derive the position-momentum uncertainty relation by using the theory of Fourier analysis. A moving particle corresponds to a single wave group. An isolated wave group is the result of superposing an infinite number of waves with different angular frequencies ω, *continuous* range of wave numbers k and amplitudes (Fig. 3.6). The composition produces oscillations confined to a *single* region of space and thus provides an idealized picture of a localized matter wave.

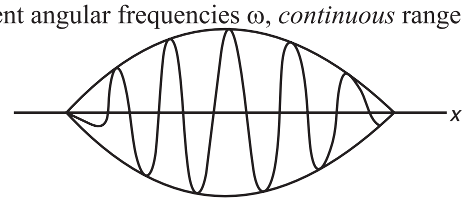


Fig. 3.6

At a certain time t, the wave group ψ (x) can be represented by the *Fourier integral*

$$\psi(x) = \int_0^\infty g(k)\cos kx\, dk$$

Here the amplitude function $g(k)$ describes how the amplitudes of the waves that contribute to ψ (x) vary with wave number k. ψ (x) and $g(k)$ are just *Fourier transforms* of each other. Fig. 7.19

shows Gaussian distributions for the amplitude function $g\ (k)$ and the wave packet $\psi\ (x)$. The relationship between the distance $\Delta\ x$ and the wave number spread $\Delta\ k$ depends upon the shape of the wave group and upon how $\Delta\ x$ and $\Delta\ k$ are defined. The widths $\Delta\ x$ and $\Delta\ k$ obey a reciprocal relation in which the product $\Delta x\ \Delta k$ is equal to pure number. The minimum value of the product $\Delta\ x\ \Delta\ k$ occurs when the envelope of the group has the bell shape of a Gaussian function (Fig. 3.7). Thus, the Gaussian wave packets happen to be minimum uncertainty wave packets. If $\Delta\ x$ and $\Delta\ k$ are taken as the standard deviations of the respective functions $\psi\ (x)$ and $g\ (k)$, then this minimum value is 1/2. Wave groups in general do not have Gaussian forms. So we can write

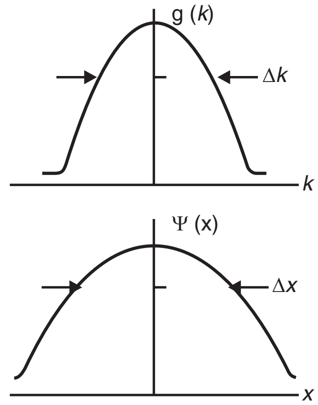


Fig. 3.7

$$\Delta x\ \Delta k \ \geq\ \frac{1}{2} \qquad \text{...(1)}$$

Let λ be the de Broglie wavelength of the particle. We see from

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

that the momentum of the particle is determined by the wave number k.

$$\therefore \qquad p = \frac{hk}{2\pi}\cdot$$

$$\Delta\ p = \frac{h\,\Delta\,k}{2\pi} = \hbar\,\Delta\,k\cdot$$

Hence an uncertainty $\Delta\ k$ in the wave number of the de Broglie waves associated with the particle results in an uncertainty $\Delta\ p$ in the particle's momentum.

From Eq. (1), $\Delta\ x\ \Delta\ k \geq 1/2$ or $\Delta\ k \geq 1/2\ \Delta\ x$

$$\therefore \qquad \Delta x\ \Delta p\ \geq\ \hbar/2 \qquad \text{...(2)}$$

This is the *Heisenberg uncertainty relation for position and momentum*.

Eq. (2) states that the product of the uncertainty Δx in the position of an object at some instant and the uncertainty Δp in its momentum component in the x direction at the same instant is equal to or greater than $\hbar/2$.

The three-dimensional form of the Heisenberg uncertainty relations for position and momentum is now

$$\Delta x\ \Delta p_x\ \geq\ \frac{\hbar}{2},\ \Delta\ y\ \Delta\ p_y \geq \frac{\hbar}{2},\ \Delta\ z\ \Delta\ p_z \geq \frac{\hbar}{2} \qquad \text{...(3)}$$

Time-Energy uncertainty relation

The theory of Fourier analysis may also be invoked to obtain a *time-energy uncertainty relation.* Indeed, according to Fourier analysis, a wave packet of duration $\Delta\ t$ must be composed of plane-wave components whose angular frequencies extend over a range $\Delta\omega$ such that $\Delta\ t\ \Delta\ \omega \geq 1/2$. Since $E = \hbar\omega$, we, therefore, have

$$\Delta t\ \Delta E \geq \hbar/2 \qquad \text{...(4)}$$

This is the *Heisenberg uncertainty relation for time and energy.* It connects the uncertainty ΔE in the determination of the energy of a system with the time interval $\Delta\ t$ available for this energy determination. Thus, if a system does not stay longer than a time $\Delta\ t$ in a given state of motion, its energy in that state will be uncertain by an amount $\Delta E \geq \hbar/2\Delta t$.

3.2.4. Elementary proof of Uncertainty Relation between Displacement and Momentum

Consider a particle in motion along the x-axis.

- The de Broglie relation between the wavelength λ of the associated wave and the momentum p_x of the particle is

$$p_x = \frac{h}{\lambda} = \hbar k \qquad ...(1)$$

Here, $k = 2\pi/\lambda$ is called the *propagation constant*.

- The particle in motion is represented by a wave-packet.

We consider the wave-packet as the superposition of two simple harmonic plane waves of propagation constant k and $k + \delta k$ (Fig. 3.8).

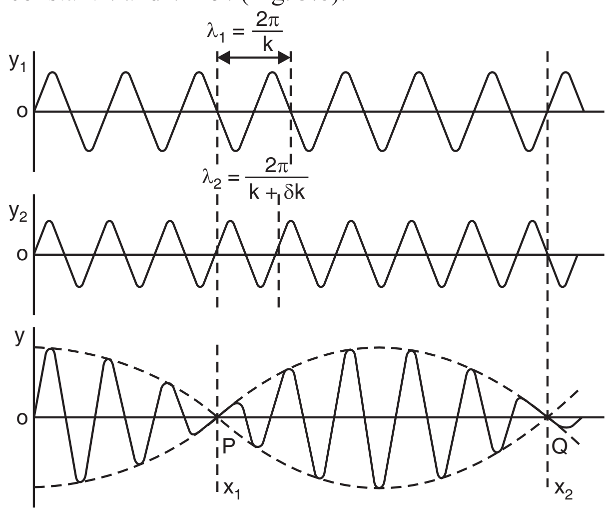


Fig. 3.8

The length of the wave-packet is

$$\Delta x = \frac{2\pi}{\Delta k} \qquad ...(2)$$

- The particle must be somewhere within the wave-packet.

Uncertainty in the position of the particle = Δx.

Uncertainty in the propagation constant = Δk.

From Eq. (1), the uncertainty Δp_x in the momentum is given by

$$\Delta p_x = \hbar\, \Delta k \qquad ...(3)$$

Multiplying Eq. (2) by Eq. (3), we get the product of the uncertainties.

$$\Delta x \,.\, \Delta p_x = \left(\frac{2\pi}{\Delta k}\right)(\hbar\, \Delta k) = 2\pi\hbar = h.$$

If wave-packets have shapes different from that shown in Fig. 3.8, then the sign of equality is replaced by the sign $\gtrsim$.

$$\therefore \qquad \Delta x \,.\, \Delta p_x \gtrsim h \qquad ...(4)$$

- A **single wave-packet** is formed by superposition of an **infinite number of plane waves** of different wave numbers k (Fig. 3.9). This wave has virtually no amplitude outside a rather narrow region of space Δx.

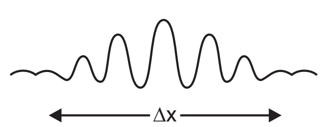


Fig. 3.9

For a **single wave-packet** Δx and Δk are related by:

$$\Delta x \gtrsim \frac{1}{\Delta k} \qquad ...(5)$$

Multiplying Eq. (3) by Eq. (5), we get

$$\Delta x \,.\, \Delta p_x \;\; \hbar \gtrsim \qquad ...(6)$$

3.2.5. Elementary Proof of the Uncertainty Relation between Energy and Time

A particle in motion is represented by a wave-packet (Fig. 3.10). Δx is the width of the wave-packet moving along the x-axis.

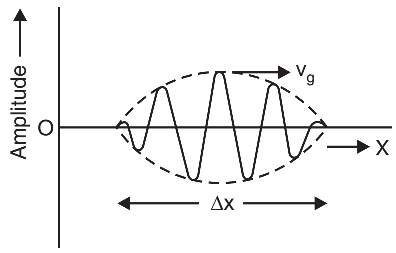


Fig. 3.10

v_g = group velocity of the wave-packet, and

v_x = particle velocity along x-axis.

The group velocity of the wave-packet is equal to the particle velocity.

$$v_g = v_x$$

Suppose the wave-packet moves through Δx in time Δt.

$$\Delta t = \frac{\Delta x}{v_g} = \frac{\Delta x}{v_x}$$

$$\therefore \qquad \Delta t = \frac{\Delta x}{v_x} \qquad ...(1)$$

Since Δx is the uncertainty in the x-coordinate of the particle, Δt is the uncertainty in time t at which the particle passes through a point with velocity v_g.

The kinetic energy of the particle, $E = \dfrac{p_x^2}{2m}$ ...(2)

Taking differential of Eq. (2), the uncertainty ΔE in the kinetic energy is given by

$$\Delta E = \frac{2 p_x \Delta p_x}{2m} = \frac{p_x}{m} \Delta p_x = \frac{m v_x}{m} \Delta p_x$$

$$\Delta E = v_x \Delta p_x \qquad ...(3)$$

Multiplying Eq. (1) by Eq. (3), we get

$$\Delta E \,.\, \Delta t = \Delta x \,.\, \Delta p_x \qquad ...(4)$$

According to the uncertainty relation between position and momentum, we have

$$\Delta x \,.\, \Delta p_x \gtrsim \hbar.$$

$\therefore$ from Eq. (4), we have

$$\Delta E \,.\, \Delta t \gtrsim \hbar \qquad ...(5)$$

This is the energy-time uncertainty relation.

3.2.6. Bohr's Complementarity Principle

Statement. *In any experimental situation in which a physical entity (matter or radiation) exhibits its wave properties, it is impossible to attribute corpuscular characteristics to it.*

- *The particle and wave aspects of a physical entity are complementary and cannot be exhibited at the same time.*

Example. In a two slit interference experiment, if we try to define electron trajectory either by closing one slit or by placing some detecting apparatus immediately behind one of the slits, the interference pattern disappears. It follows that any experiment which can be devised either displays wave like or particle like characteristics of the system. The wave and particle pictures give complementary descriptions of the same system.

Illustration. Consider an experimental arrangement in which light is diffracted by a double slit and is detected on a screen (Fig. 3.11). Suppose the light beam is very weak and there is only one photon at a time in the apparatus. We can regard each photon as having a wave associated with it. The two slits transmit the photon in the manner of a wave passing through *both* slits at once. When it strikes the screen, light is behaving as a particle does. Thus the wave and particle pictures give complementary descriptions of the same system. Bohr introduced the **complementarity principle.**

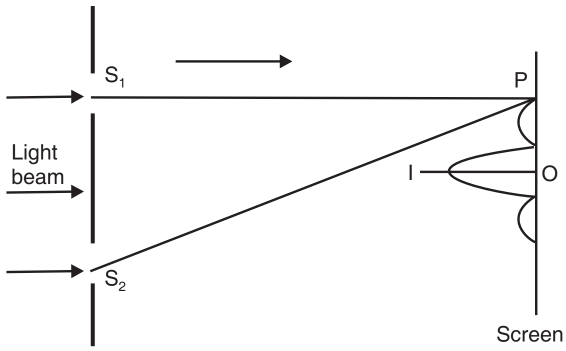


Fig. 3.11

It states that the wave and particle aspects of matter are complementary rather than being contradictory, both equally essential for a full description of the phenomenon.

EXERCISE

1. The de Broglie wavelength of a particle of mass *m* and momentum *p* is given by

(*a*) $\lambda = \frac{h}{p}$ (*b*) $\lambda = \frac{p}{h}$ (*c*) $\lambda = \frac{h}{2p}$ (*d*) $\lambda = \frac{2p}{h}$

2. If the momentum of a particle is doubled, then its de Broglie wavelength

(*a*) zero (*b*) halves (*c*) double (*d*) unchanged.

3. De-Broglie wavelength for thermal neutrons

(*a*) $\lambda = \frac{h}{3mkT}$ (*b*) $\lambda = \frac{h}{\sqrt{2mkT}}$ (*c*) $\lambda = \frac{h}{mkT}$ (*d*) $\lambda = \frac{h}{\sqrt{mkT}}$.

4. The group velocity is given by

(*a*) $v_g - v_p$ (*b*) $v_g = \lambda v_p$ (*c*) $v_g = v_p - \lambda \frac{dv_p}{d\lambda}$ (*d*) $v_g = v_p - \frac{dv_p}{d\lambda}$.

5. The phase velocity of de Broglie wave

(*a*) $v_p = \frac{v}{c}$ (*b*) $v_p = \frac{c}{v}$ (*c*) $v_p = \frac{c^2}{v}$ (*d*) $v_p = \frac{v}{c^2}$.

6. Which one of the following is true?

(a) $\Delta J \, \Delta\theta \geq \hbar$ b) $\Delta J \, \Delta x \geq (\hbar$ (*c*) $\Delta J \, \Delta p \geq h$ (*d*) $\Delta J \, \Delta k \geq \hbar$

Ans. 1. (*a*), **2.** (*b*), **3.** (*b*), **4.** (*c*), **5.** (*c*), **6.** (*a*)

7. Explain the concept of matter waves.

8. Derive de Broglie relation for matter waves.

9. Derive an expression for phase velocity.

10. Derive an expression for group velocity.

11. Show that the group velocity of the de-Broglie wave associated with a particle is the same as the particle velocity.

13. State Heisenberg's uncertainty principle and give two illustrations.

14. Derive Heisenberg uncertainty relation.

15. Explain the concept of energy and time uncertainty.

16. Explain non-existence of free electrons in the nucleus.

17. 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.

Solution. We have, $\Delta E \, \Delta t \geq \hbar$

$$\therefore \quad \Delta E \geq \frac{\hbar}{\Delta t} = \frac{1.055 \times 10^{-34}}{(10^{-8})}$$

$$\therefore \quad \Delta E \geq 1.0 \times 10^{-26} \text{ J} = 6.5 \times 10^{-8} \text{ eV.}$$

This is known as the *energy width* of an excited state.

20. 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?

[**Hint:** $\Delta x \, \Delta p \sim \hbar$. Given: $\Delta x = 0.2 \times 10^{-10}$ m

$\Delta p \sim 5.27 \times 10^{-24}$ kg m/s]

UNIT IV

OPERATORS AND SCHRÖDINGER EQUATION

Postulates of quantum mechanics. Wave functions and its interpretation – linear operators – Eigenvalue – Hermitian operator – Properties of Hermitian operator – Commutator Algebra. SCHRÖDINGER EQUATION: Schrödinger's wave equation in time dependent form – Steady state Schrödinger's wave equation – extension to three dimensions.

4.1. POSTULATES OF QUANTUM MECHANICS

Postulate 1 – The State

The state of a system is described by a wave function $\psi(\mathbf{r}, t)$.

Explanation. For a single particle, the *wave-function* is a function only of position **r** and time t, and is written $\psi(\mathbf{r}, t)$. The wave function $\psi(\mathbf{r}, t)$ gives the complete knowledge of the behaviour of the particle

Similarly, $\psi(\mathbf{r})$ gives the stationary state which is independent of time.

- The wave function is a complex function of co-ordinates and time.

  The probability of finding the particle in the space within r and $r + dr$ is $\psi^* \psi \, dr$.

- In order to conform to the physically realisable states, it must be well- behaved, *i.e.*, it must be singled-valued, continuous and finite.

Postulate 2 – Operators

Every physical observable is associated with a linear Hermitian operator.

Explanation. The result of measurements is a number. The eigenvalues of a *Hermitian operator* are real, which justifies their use.

- The *linearity* condition stems from the superposition principle.

Statement of Superposition Principle

If any system (a particle or an assembly of particles) can exist in a state represented by the wave function Ψ_1 and also in a state represented by the wave function Ψ_2, then it can be also in a state represented by a wave function Ψ such that

$$\Psi = c_1\Psi_1 + c_2\Psi_2.$$

Here, c_1 and c_2 are arbitrary, in general, complex numbers.

- In quantum mechanics, dynamical variables like position, momentum, angular momentum, energy, etc., are called 'Observables'. The observables are represented by **hermitian operators**.

Hermitian Operators naturally arise in quantum mechanics because their expectation values are real. Table 10.1 lists the operators that correspond to various observable quantities.

TABLE 4.1. Operators Associated with Various Observable Quantities

Quantity	Operator
Position, x	x
Linear momentum, p	$-i\hbar\dfrac{\partial}{\partial x}$ (or) $-i\hbar\nabla$
Angular momentum, $\mathbf{r} \times \mathbf{p}$	$-i\hbar\, \mathbf{r} \times \nabla$
Kinetic energy, KE = $\dfrac{p^2}{2m}$	$-\dfrac{\hbar}{2m}\dfrac{\partial^2}{\partial x^2}$ (or) $-\dfrac{\hbar^2}{2m}\nabla^2$
Total energy, E	$i\hbar\dfrac{\partial}{\partial t}$
Total energy (Hamiltonian form), H	$-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V(x)$ (or) $-\dfrac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$

Linear Operator. An operator transforms one function into another. A well-known example is the differential operator $D = d/dx$, *e.g.*, $Dx^3 = 3x^2$.

In quantum mechanics, we are concerned with linear operators.

An operator α is said to be linear if

$$\alpha(\psi_1 + \psi_2) = \alpha\,\psi_1 + \alpha\,\psi_2 \text{ and } \alpha\,(a\,\psi) = a\,\alpha\,\psi.$$

ψ_1 and ψ_2 are arbitrary functions. a is a constant which may or may not be complex.

The operator D is linear.

Definition of Operator. An operator is defined as a rule by which a given function is transformed into another function.

An *operator* tells us what operation to carry out on the quantity that follows it. Thus the operator $i\hbar\frac{\partial}{\partial t}$ instructs us to take the partial derivative of what comes after it with respect to t and multiply the result by $i\hbar$.

Postulate 3 – Eigenvalues

The only possible values which a measurement of the observable (*whose operator is* α) *can yield are the eigen values* a_n *of the equation*

$$\alpha\,\psi_n = a_n\,\psi_n. \quad n = 1, 2, 3, \ldots$$

This is true provided $\int \psi_n^* \, \psi_n \, d\tau < \infty$ and ψ_n is single-valued.

- The eigenfunctions ψ_n form a complete set of n independent functions.
- The eigenvalues a_n are just numbers.

An experiment always gives a real number. Hence, the eigenvalues have to be real.

Since Hermitian operators have real eigenvalues, the operators associated with physical quantities must be Hermitian.

Example. *An eigenfunction of the operator* $\frac{d^2}{dx^2}$ *is* $\psi = e^{2x}$. *Find the corresponding eigenvalue.*

Sol. The eigenvalue equation is $\mathbf{G}\,\psi_n = G_n\,\psi_n$.

Here, $\mathbf{G}$ is the operator that corresponds to a certain dynamical variable G and each G_n is a real number.

$$\mathbf{G}\psi = \frac{d^2}{dx^2}(e^{2x}) = 4e^{2x} = 4\psi \qquad (\because\ e^{2x} = \psi)$$

$$\therefore \qquad \mathbf{G}\psi = 4\psi.$$

The eigenvalue is $G = 4$.

Postulate 4 – Expectation Values

The average value of an observable a, corresponding to the operator α, *for a system described by the wave function* ψ *is given by*

$$< a > = \frac{\int \psi^* \alpha\, \psi\, d\tau}{\int \psi^* \psi\, d\tau}.$$

The quantity $< a >$ is called the *expectation value*.

- If the wave function is normalised, the denominator is unity. We can write

$$< a > = \int \psi^* \alpha \, \psi \, d\tau$$

- The first four postulates deal with the properties of the quantum system at any given instant of time.

Postulate 5 – Time development of a quantum system

The development in time of the wave function ψ of a system is given by the equation.

$$\hat{H}\psi = i\hbar \frac{\partial}{\partial t}\psi \, .$$

Here, $\hat{H}$ is the *Hamiltonian operator*.

This postulate is simply a statement of the time dependent Schrodinger equation. If the wave function is known at some initial time, the above equation determines ψ at any other time.

- The time development of state, *i.e.*, how the state changes as time progresses, is given by the Schrodinger equation.

OPERATORS IN QUANTUM MECHANICS

4.1.1. Operator for Momentum

The wave function for a free particle moving in the positive *x*-direction is

$$\psi(x, t) = Ae^{i/\hbar\,(p_x x - Et)} \quad \text{...(1)}$$

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

$$\frac{\partial \psi}{\partial x} = A\left(\frac{i}{\hbar}\right)p_x \, e^{i/\hbar\,(p_x x - Et)} = \frac{i}{\hbar}p_x\psi$$

$$\frac{\hbar}{i}\frac{\partial \psi}{\partial x} = p_x \, \psi$$

$$-i\hbar\frac{\partial \psi}{\partial x} = p_x \, \psi \quad \text{...(2)}$$

Eq. (2) is the eigen value equation for the *x*-component of the momentum.

- $-i\hbar\frac{\partial}{\partial x}$ is the operator.
- ψ (*x*, *t*) is the *eigen function* of the operator.
- p_x is the *eigen value* of the operator.

∴ $-i\hbar\frac{\partial}{\partial x}$ is the operator for the *x*-component of the momentum. Thus

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \quad \text{...(3)}$$

Similarly, for the *y* and *z*-components of the momentum, the operators are

$$\hat{p}_y = -i\hbar\frac{\partial}{\partial y} \quad \text{...(4)}$$

$$\hat{p}_z = -i\hbar\frac{\partial}{\partial z} \quad \text{...(5)}$$

In three dimensions, the operator for the momentum **p** is

$$\hat{p} = -i\hbar \, \nabla \quad \text{...(6)}$$

Example 1. *Find the eigen values of the linear momentum operator.*

Sol. The eigenvalue equation of linear momentum is

$$-i\hbar\frac{d\psi}{dx} = a\psi; \ (a = \text{eigenvalue})$$

$$\frac{d\psi}{\psi} = \frac{ia}{\hbar}dx$$

Integrating,
$$\ln\psi = \frac{ia}{\hbar}x + \ln C; \ \ C = \text{constant}$$

$\therefore$
$$\psi = C\exp\left(\frac{ia}{\hbar}x\right)$$

For ψ to be finite in the region $-\infty$ to $+\infty$, the eigenvalue a has to be real. Hence, all real values of a are the eigenvalues of linear momentum. In other words, linear momentum is not quantized.

4.1.2. Operator for Kinetic Energy

From the momentum operator, we have

$$-i\hbar\frac{\partial\psi}{\partial x} = p_x\psi \qquad ...(1)$$

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

$$-i\hbar\frac{\partial^2\psi}{\partial x^2} = p_x\frac{\partial\psi}{\partial x}$$

But,
$$\frac{\partial\psi}{\partial x} = \frac{1}{-i\hbar}p_x\psi$$

$\therefore$
$$-i\hbar\frac{\partial^2\psi}{\partial x^2} = p_x\left(\frac{1}{-i\hbar}\right)p_x\psi$$

or
$$-\hbar^2\frac{\partial^2\psi}{\partial x^2} = p_x^2\psi \qquad ...(2)$$

Dividing Eq. (2) by $2m$, we get

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p_x^2}{2m}\psi$$

or
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = K\psi \qquad ...(3)$$

Here,
$$K = \frac{p_x^2}{2m} = \text{kinetic energy of the particle.}$$

Eq. (3) is the eigen value equation for the kinetic energy of the particle moving in the x-direction.

- $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ is the operator.
- $\psi(x, t)$ is the eigen function of the operator.
- $K = \frac{p_x^2}{2m}$ is the eigen value of the operator.

$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ is the kinetic energy operator for the motion of the particle in the x-direction.

$$\therefore \qquad \hat{K} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad ...(4)$$

In three dimensions, the operator for kinetic energy is

$$\hat{K} = -\frac{\hbar^2}{2m}\nabla^2 \qquad ...(5)$$

4.1.3. Operator for Total Energy

The total energy of a particle moving in the x-direction is given by

$$E = \frac{p_x^2}{2m} + V(x) \qquad ...(1)$$

Here, $V(x)$ is the potential energy.

or
$$\frac{p_x^2}{2m} + V = E$$

Multiplying through by $\psi(x, t)$, we get

$$\frac{p_x^2}{2m}\psi + V\psi = E\psi$$

But
$$\frac{p_x^2}{2m}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

$$\therefore \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\psi = E\psi \qquad ...(2)$$

Eq. (2) is the eigen value equation for the total energy E of the particle moving in the x-direction.

- $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$ is the operator.
- $\psi(x, t)$ is the eigen function of the operator.
- E is the eigen value of the operator.

$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$ is the total energy operator for the motion of the particle along the x-direction.

$$\hat{H}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \qquad ...(3)$$

$\hat{H}_x$ is called the Hamiltonian operator for one-dimensional motion.

For three-dimensional motion, the total energy operator is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \qquad ...(4)$$

Here, $$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$\hat{H}$ is called the *Hamiltonian operator*.

4.1.4. Operator for Total Energy in terms of Partial Derivative with respect to Time

The wave function for a free particle moving in the positive x-direction is

$$\psi(x, t) = A\, e^{i/\hbar\,(p_x x - Et)} \quad ...(1)$$

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

$$\frac{\partial \psi}{\partial t} = A\left(\frac{i}{\hbar}\right)(-E)\, e^{(i/\hbar)(p_x x - Et)}$$

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

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} E\psi$$

or $$i\hbar \frac{\partial}{\partial t}\psi = E\psi \quad ...(2)$$

Evidently the dynamical quantity E in some sense corresponds to the differential operator $i\hbar \frac{\partial}{\partial t}$.

The total – energy operator is

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \quad ...(3)$$

4.1.5. Orbital Angular Momentum Operator

The classical orbital angular momentum of a particle is

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad ...(1)$$

where **r** and **p** are the position and momentum vectors of the particle, respectively. **p** is represented by the vector operator $-i\hbar\nabla$. So **L** is represented by the vector operator $-i\,\hbar(\mathbf{r} \times \nabla)$.

$$\mathbf{L} = \mathbf{r} \times (-i\hbar\, \nabla) = -i\hbar\, \mathbf{r} \times \nabla \quad ...(2)$$

Let L_x, L_y, L_z be cartesian components of **L.**

$$\mathbf{i}\, L_x + \mathbf{j}\, L_y + \mathbf{k}\, L_z = -i\hbar \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix}$$

$$\therefore \quad \hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \quad ...(3)$$

Let us now represent Cartesian components L in terms of spherical polar coordinates. The Cartesian coordinates (x, y, z) and spherical polar coordinates (r, θ, ϕ), are related by Fig. 4.1.

$$x = r\sin\theta\cos\phi,$$
$$y = r\sin\theta\sin\phi,$$
$$z = r\cos\theta. \qquad ...(1)$$

These equations yield

$$r^2 = x^2 + y^2 + z^2, \cos\theta = \frac{z}{r}.$$
$$\tan\phi = \frac{y}{x} \qquad ...(2)$$

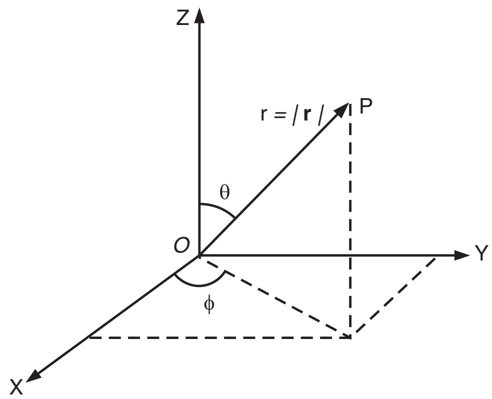


Fig. 4.1

Using Eqs. (1) and (2), we obtain

$$\frac{\partial r}{\partial x} = \sin\theta\cos\phi, \frac{\partial r}{\partial y} = \sin\theta\sin\phi, \frac{\partial r}{\partial z} = \cos\theta$$
$$\frac{\partial \theta}{\partial x} = \frac{1}{r}\cos\theta\cos\phi, \frac{\partial \theta}{\partial y} = \frac{1}{r}\cos\theta\sin\phi, \frac{\partial \theta}{\partial z} = -\frac{1}{r}\sin\theta \qquad ...(3)$$
$$\frac{\partial \phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta}, \frac{\partial \phi}{\partial y} = \frac{\cos\phi}{r\sin\theta}, \frac{\partial \phi}{\partial z} = 0.$$

Using these relations, we obtain

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}$$
$$= \sin\theta\cos\phi\frac{\partial f}{\partial r} + \frac{1}{r}\cos\theta\cos\phi\frac{\partial f}{\partial \theta} - \left(-\frac{1}{r}\frac{\sin\phi}{\sin\theta}\frac{\partial f}{\partial \phi}\right) \qquad ...(4)$$
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial y} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial y}$$
$$= \sin\theta\sin\phi\frac{\partial f}{\partial r} + \frac{1}{r}\cos\theta\sin\phi\frac{\partial f}{\partial \theta} + \frac{1}{r}\frac{\cos\phi}{\sin\theta}\frac{\partial f}{\partial \phi}. \qquad ...(5)$$
$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial z} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial z} = \cos\theta\frac{\partial f}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial f}{\partial \theta}. \qquad ...(6)$$
$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial \theta} + \cot\theta\cos\phi\frac{\partial}{\partial \phi}\right) \qquad ...(7)$$
$$L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial \theta} + \cot\theta\sin\phi\frac{\partial}{\partial \phi}\right) \qquad ...(8)$$
$$L_z = -i\hbar\frac{\partial}{\partial \phi}. \qquad ...(9)$$

L^2 in spherical polar coordinates is given by

$$L^2 = L_x^2 + L_y^2 + L_z^2$$
$$= -\hbar^2\left[\left\{\sin^2\phi\frac{\partial^2}{\partial \theta^2} + \cot^2\theta\cos^2\phi\frac{\partial^2}{\partial \phi^2} + \sin\phi\frac{\partial}{\partial \theta}\left(\cot\theta\cos\phi\frac{\partial}{\partial \phi}\right)\right.\right.$$

$$+\cot\theta\cos\phi\frac{\partial}{\partial\phi}\left(\sin\phi\frac{\partial}{\partial\theta}\right)\Bigg\}+\Bigg\{\cos^2\phi\frac{\partial^2}{\partial\theta^2}+\cot^2\theta\sin^2\phi\frac{\partial^2}{\partial\phi^2}$$

$$-\cos\phi\frac{\partial}{\partial\theta}\left(\cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)+\cot\theta\sin\phi\frac{\partial}{\partial\phi}\left(-\cos\phi\frac{\partial}{\partial\theta}\right)\Bigg\}+\left\{\frac{\partial^2}{\partial\phi^2}\right\}\Bigg]$$

$$= -\hbar^2\left[\frac{\partial^2}{\partial\theta^2}+(\cot^2\theta+1)\frac{\partial^2}{\partial\phi^2}+\sin\phi(-\mathrm{cosec}^2\,\theta)\cos\phi\frac{\partial}{\partial\phi}\right.$$

$$\left.+\cot\theta\cos^2\phi\frac{\partial}{\partial\theta}-\cos\phi(-\mathrm{cosec}^2\,\theta)\sin\phi\frac{\partial}{\partial\phi}+\cot\theta\sin^2\phi\frac{\partial}{\partial\theta}\right]$$

$$= -\hbar^2\left[\frac{\partial^2}{\partial\theta^2}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+\cot\theta\frac{\partial}{\partial\theta}\right]$$

$$= -\hbar^2\left[\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}+\frac{\partial^2}{\partial\theta^2}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

$$\therefore \qquad \mathbf{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \qquad ...(10)$$

This is the expression for the operator of the square of the angular momentum.

Expressions for the Eigen values of the square of the total angular momentum ($\mathbf{L}^2$) and its *z*-component ($\mathbf{L}_z$).

The angular momentum of atoms and molecules is almost as important as the energy as it helps to give physical significance to our mathematical functions. For a one-electron atom, the angular momentum **L** is quantized both in magnitude and direction, with relations

$$|\mathbf{L}|^2 = l(l+1)\hbar^2$$

and $$L_z = m_l\hbar.$$

Here, $|\mathbf{L}|^2$ is the square of the magnitude of the orbital angular momentum about the centre of the atom and L_z is the component of the angular momentum along the z-axis.

l and m_l are quantum numbers which restrict $|\mathbf{L}|^2$ and L_z to certain specific values.

To prove the above relations for an atom we must show that the wave functions of the atom are eigenfunctions of the angular momentum operators $\hat{\mathbf{L}}^2$ and $\hat{\mathbf{L}}_z$ with eigenvalues $l(l+1)\hbar^2$ and $m_l\hbar$ respectively.

Let us now first apply the operator $\hat{L}_z$ to the one-electron atom wave function

$$\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

$$\hat{L}_z\psi = -i\hbar\frac{\partial\psi}{\partial\phi}$$

or $$L_z\psi = -i\hbar R\,\Theta\frac{d\Phi}{d\phi}$$

The function $\Phi(\phi)$ for the atom is given by

$$\Phi = Ae^{im_l\phi}$$

$$\frac{d\Phi}{d\phi} = Aim_l e^{im_l\phi} = im_l\Phi.$$

Substituting it in the above expression for $\hat{L}_z \psi$, we get

$$\hat{L}_z \psi = -i\hbar \, im_l R \Theta \Phi$$

or

$$\hat{L}_z \psi = m_l \hbar \psi$$

This result means that the wave functions ψ of the one-electron atom are the eigen functions of $\hat{L}_z$ having eigen values given by

$$L_z = m_l \hbar. \qquad ...(4)$$

This is the expression for the quantized values of the *z*-component of the angular momentum of the atom. (L_x and L_y, however, do *not* obey quantization relations).

We next apply the operator $\hat{\mathbf{L}}^2$ to the wave function $\psi = R\,\Theta\,\Phi$.

$$\hat{L}^2 \psi = -\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] R\Theta\Phi \qquad ...(5)$$

$$= -\hbar^2 \, R\left[\frac{\Phi}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{\Theta}{\sin^2\theta}\frac{d^2\Phi}{d\phi^2}\right].$$

The Φ-equation is $\Phi = Ae^{im_l \Phi}$

$$\frac{d^2\Phi}{d\phi^2} = A(im_l)^2 e^{im_l \Phi} = -m_l^2 \Phi.$$

$$\therefore \qquad \hat{L}^2 \psi = -\hbar^2 R\Phi\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\frac{m_l^{\,2}}{\sin^2\theta}\Theta\right].$$

The function Θ (θ) is a solution of the equation

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)-\frac{m_l^2}{\sin^2\theta}\right]\Theta = 0.$$

This means that the quantity in brackets in the above expression for $\hat{L}^2 \psi$ is equal to $-l(l+1)\Theta$. Hence we get

$$\hat{L}^2 \psi = -\hbar^2 R \Phi [-l(l+1)\Theta]$$

or

$$\hat{L}^2 \psi = l(l+1)\hbar^2 R \Theta \Phi$$

or

$$\hat{L}^2 \psi = l(l+1)\hbar^2 \psi$$

It means that the wave functions ψ of the one-electron atom are the eigenfunctions of $\hat{L}^2$ having eigenvalues given by

$$|\mathbf{L}|^2 = l(l+1)\hbar^2$$

This is the expression for the quantized values of the square of the angular momentum of the atom.

4.2. COMMUTING OPERATORS

- If $\hat{A}\hat{B} = \hat{B}\hat{A}$, $\hat{A}$ *and* $\hat{B}$ are said to commute.
- If $\hat{A}\hat{B} \neq \hat{B}\hat{A}$, $\hat{A}$ *and* $\hat{B}$ are said not to commute.

Example. If $\hat{A} = x$ and $\hat{B} = \frac{d}{dx}$ then,

$$\hat{A}\hat{B}\psi = x\frac{d\psi}{dx}$$

$$\hat{B}\hat{A}\psi = \frac{d}{dx}(x\psi)$$

$$= \psi + x\frac{d\psi}{dx}$$

Hence $\hat{A}\hat{B}\psi \neq \hat{B}\hat{A}\psi$

or $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

In the special case if $\hat{A}\hat{B} = \hat{B}\hat{A}$, then the operators A and B are said to commute.

- The difference $AB - BA$ is called the commutator of A and B.
- A bracket notation is used to denote the commutator

$$[A, B] \equiv AB - BA.$$

- When two operators commute, it is possible to measure both the variables associated with them simultaneously and accurately. Further, there will be no uncertainty in either of them.
- If two operators do not commute, it is not possible to measure the variables associated with them simultaneously and accurately. If one of them is measured accurately, it is not possible to measure the other simultaneously with accuracy.

4.2.1. Simultaneous eigenfunctions

If A and B are linear operators, and ψ is a function satisfying both the equations

$$A\psi = \alpha\psi, \quad B\psi = \beta\psi, \qquad ...(1)$$

then ψ is a *simultaneous* eigenfunction of A and B, belonging to the eigenvalues α and β, respectively.

For example, consider a nonrelativistic free particle, of energy $E = \frac{1}{2}mv^2$ and momentum $p = mv$. The wave function

$$\psi_p = \frac{1}{\sqrt{2\pi\hbar}} e^{(i/\hbar)px}, \qquad ...(2)$$

satisfies simultaneously the equations

$$\hat{p}\,\psi = p\psi \quad \text{and} \quad \hat{H}\,\psi = E\psi.$$

Here, $\hat{H} = \frac{\hat{p}^2}{2m}$ is the Hamiltonian operator for a free particle.

Equations (1) imply that

$$B\,A\psi = B(\alpha\psi) = \alpha B\psi = \alpha\beta\psi,$$

and $$A\,B\psi = A(\beta\psi) = \beta\,A\psi = \beta\alpha\psi.$$

By subtraction,

$$(AB - BA)\,\psi = 0. \qquad ...(3)$$

This equation shows that ψ is also an eigenfunction of the operator $(AB - BA)$, belonging to the eigenvalue zero. The condition (3) is necessary in order that ψ be a simultaneous eigenfunction of A and B.

The operator in Eq. (3) is called the *commutator* of A and B and is written,

$$[A, B] = AB - BA. \qquad ...(4)$$

Two operators satisfying the equation

$$[A, B] = 0 \qquad ...(5)$$

are said to *commute.* This equation means that Eq. (3) is true for every ψ which is a member of the class of functions under consideration.

The eigenfunctions of commuting operators can always be constructed in such a way that they are simultaneous eigenfunctions.

4.2.2. Simultaneous Measurability of Observables

If two observables are simultaneously measurable in a particular state of a given system, then the state function is an eigenfunction of both the operators. Two observables are said to be *compatible,* if their operators have a common set of eigenfunctions. The following two theorems indicate the connection between compatible observables and commuting operators.

Theorem 1. *Operators having common set of eigenfunctions commute.*

Proof. Consider operators A and B with the common set of eigenfunctions ψ_i, $i = 1, 2, ...$ as

$$A\psi_i = a_i \psi_i, \quad \text{and} \quad B\psi_i = b_i\psi_i \qquad ...(1)$$

Then
$$AB\psi_i = A(b_i\psi_i) = b_iA\psi_i = a_ib_i\psi_i \qquad ...(2)$$
and
$$BA\psi_i = B(a_i\psi_i) = a_iB\psi_i = a_ib_i\psi_i \qquad ...(3)$$

Since $AB\psi_i = BA\psi_i$, A commutes with B. Hence the result.

Theorem 2. *Commuting operators have common set of eigenfunctions.*

Proof. Consider two commuting operators A and B. The eigenvalue equation for A is

$$A\psi_i = a_i\psi_i, \quad i = 1, 2, \qquad ...(1)$$

Operating both sides from left by B, we get

$$BA\psi_i = a_iB\psi_i$$

Since B commutes with A,

$$A(B\psi_i) = a_i(B\psi_i) \qquad ...(2)$$

That is, $B\psi_i$ is an eigenfunction of A with the same eigenvalue a_i. If A has only nondegenerate eigenvalues, $B\psi_i$ can differ from ψ_i only by a multiplicative constant, say b_i

$$B\psi_i = b_i\psi_i \qquad ...(3)$$

In other words, ψ_i is a simultaneous eigenfunction of both A and B.

Explanaton of the Two Theorems (Theorem of commutativity and simultaneity)

Theorem. *If two operators A and B possess a complete set of simultaneous eigen functions, then the operators A and B commute, i.e.,*

$$AB = BA \quad \text{or} \quad AB - BA = 0 \quad \text{or} \quad [A, B] = 0.$$

Converse of theorem

The converse of the theorem is stated as follows:

Theorem. *If two operators commute, they possess a set of simultaneous eigen functions.*

4.2.3. Commutator Algebra

We list here some elementary rules for the calculation of commutators.

If A, B, and C are three linear operators

$$[A, B] = -[B, A] \qquad ...(1)$$

$$[A, B + C] = [A, B] + [A, C] \qquad ...(2)$$

$$[A, BC] = [A, B]C + B[A, C] \quad ...(3)$$
$$[AB, C] = [A, C]B + A[B, C] \quad ...(4)$$
$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \quad ...(5)$$

Now, let us simplify $[A, [B, C]]$.

$$[A, [B, C]] = A[B, C] - [B, C]A$$
$$= A(BC - CB) - (BC - CB)A$$
$$= ABC - ACB - BCA + CBA.$$

(*a*) Commutation relation between position and momentum

(*i*) Let x and p_x be represented as

$$x \to \hat{x},\ p_x \to \hat{p}_x = -i\hbar\frac{\partial}{\partial x}.$$

Consider a function $\psi(x)$. Then

$$p_x \psi = -i\hbar\frac{\partial \psi}{\partial x}$$

and
$$xp_x \psi = x\left(-i\hbar\frac{\partial \psi}{\partial x}\right) \quad ...(1)$$

Also
$$p_x x\psi = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar\psi + x\left(-i\hbar\frac{\partial \psi}{\partial x}\right) \quad ...(2)$$

Eq. (1) – Eq. (2) gives,

$$xp_x\psi - p_x x\psi = x\left(-i\hbar\frac{\partial \psi}{\partial x}\right) - \left[-i\hbar\psi + x\left(-i\hbar\frac{\partial \psi}{\partial x}\right)\right] = i\hbar\psi$$

$\therefore$
$$[x, p_x] = i\hbar \quad ...(3)$$

Now,
$$p_y = -i\hbar\frac{\partial}{\partial y} \text{ and } p_z = -i\hbar\frac{\partial}{\partial z}.$$

We have proved the relation $[x, p_x] = i\hbar$.

More generally, we have

$$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar. \quad ...(4)$$

while all other commutators such as $[x, p_y]$ – vanish. It follows that, for example, x and p_y have common eigenfunctions and can be measured simultaneously with arbitrary accuracy. In contrast, since x and p_x do not commute with each other, a precise simultaneous measurement of both of these observables is impossible.

(*ii*) $[x^2, p_x] = [xx, p_x] = [x, p_x]x + x[x, p_x] = i\hbar x + xi\hbar = 2i\hbar x.$

(*b*) Commutation relation between Hamiltonian H and momentum p

The Hamiltonian operator for free particle is

$$\hat{H}_x = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \text{ since potential energy } V = 0$$

and
$$\hat{p}_x = -i\hbar\frac{d}{dx}.$$

Consider a function $\psi(x)$. Then,

$$p\psi = -i\hbar\frac{d\psi}{dx}$$

$\therefore \qquad Hp\,\psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(-i\hbar\frac{d\psi}{dx}\right).$

Similarly, $\qquad pH\,\psi = -i\hbar\frac{d}{dx}\left[-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\right]$

Solving, $[H, p] = Hp - pH = 0$,

i.e., momentum of a free particle commutes with the Hamiltonian operator.

(*c*) The commutation rules for the components of orbital angular momentum (*L*)

Let L_x, L_y, L_z be cartesian components of $\boldsymbol{L}$.

$$\left.\begin{aligned}\hat{L}_x &= -i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)\\ \hat{L}_y &= -i\hbar\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)\\ \hat{L}_z &= -i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\end{aligned}\right\} \qquad \text{...(1)}$$

Now, $\qquad [L_x, L_y] = L_x L_y - L_y L_x.$

Substituting operator values

$$\begin{aligned}L_x L_y &= (-i\hbar)^2\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)\\ &= -\hbar^2\left\{y\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial x}\right)-y\frac{\partial}{\partial z}\left(x\frac{\partial}{\partial z}\right)-z\frac{\partial}{\partial y}\left(z\frac{\partial}{\partial x}\right)+z\frac{\partial}{\partial y}\left(x\frac{\partial}{\partial z}\right)\right\}\\ &= -\hbar^2\left\{y\frac{\partial}{\partial x}+yz\frac{\partial^2}{\partial z\,\partial x}-yx\frac{\partial^2}{\partial z^2}-z^2\frac{\partial^2}{\partial y\,\partial x}+zx\frac{\partial^2}{\partial y\,\partial z}\right\}\end{aligned}$$

Similarly,

$$\begin{aligned}L_y L_x &= -\hbar^2\left\{\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)\right\}\\ &= -\hbar^2\left\{z\frac{\partial}{\partial x}\left(y\frac{\partial}{\partial z}\right)-z\frac{\partial}{\partial x}\left(z\frac{\partial}{\partial y}\right)-x\frac{\partial}{\partial z}\left(y\frac{\partial}{\partial z}\right)+x\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial y}\right)\right\}\\ &= -\hbar^2\left\{zy\frac{\partial^2}{\partial x\,\partial z}-z^2\frac{\partial^2}{\partial x\,\partial y}-xy\frac{\partial^2}{\partial z^2}+x\frac{\partial}{\partial y}+xz\frac{\partial^2}{\partial z\,\partial y}\right\}\end{aligned}$$

But $\qquad \frac{\partial^2}{\partial x\,\partial z} = \frac{\partial^2}{\partial z\,\partial x}$ and $\frac{\partial^2}{\partial y\,\partial z} = \frac{\partial^2}{\partial z\,\partial y}$ and so on.

$\therefore \qquad L_x L_y - L_y L_x = [L_x, L_y] = -\hbar^2\left\{y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right\}$

Thus

$$\begin{aligned}[L_x, L_y] &= -i\hbar\left\{-i\hbar\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)\right\}\\ &= i\hbar\left\{-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\right\}\end{aligned}$$

$$[L_x, L_y] = i\hbar\, L_z \qquad \text{...(2)}$$

$\hat{L}_x, \hat{L}_y, \hat{L}_z$ do not commute with one another.

$$[\hat{L}_x, \hat{L}_y] = i\hbar\, \hat{L}_z\, ; [\hat{L}_y, \hat{L}_z] = i\hbar\, \hat{L}_x\, ;\ [\hat{L}_z, \hat{L}_x] = i\hbar\, \hat{L}_y$$

(*d*) Commutation relation of L^2 with components L_x, L_y and L_z

We have, $L^2 = L_x^2 + L_y^2 + L_z^2$

$$\begin{aligned}
[L^2, L_x] &= [L_x^2 + L_y^2 + L_z^2, L_x] \\
&= (L_x^2 + L_y^2 + L_z^2)\, L_x - L_x\, (L_x^2 + L_y^2 + L_z^2) \\
&= L_x^2 L_x + L_y^2\, L_x + L_z^2 L_x - (L_x L_x^2 + L_x L_y^2 + L_x L_z^2) \\
&= (L_y^2 L_x - L_x L_y^2) + (L_z^2 L_x - L_x L_z^2) \\
&= [L_y^2, L_x] + [L_z^2, L_x]
\end{aligned}$$

We know that

$$[AB, C] = [A, C]\, B + A\, [B, C]$$

So,

$$\begin{aligned}
[L^2, L_x] &= [L_y L_y, L_x] + [L_z L_z, L_x] \\
&= [L_y, L_x]\, L_y + L_y\, [L_y, L_x] + [L_z, L_x]\, L_z + L_z\, [L_z, L_x]
\end{aligned}$$

Now, $[L_x, L_y] = i\hbar\, L_z;\ [L_y, L_x] = -i\hbar\, L_z;\ [L_z, L_x] = i\hbar\, L_y.$

$\therefore$ $[L^2, L_x] = (-i\hbar\, L_z)\, L_y + L_y\, (-i\hbar\, L_z) + (i\hbar\, L_y)\, L_z + L_z\, (i\hbar\, L_y) = 0.$

$\therefore$ $[L^2, L_x] = 0$ ...(1 *a*)

Similarly, $[L^2, L_y] = 0$ ...(1 *b*)

$[L^2, L_z] = 0$ ...(1 *c*)

Hence L^2 commutes with any of the three components of the angular momentum operator.

(*e*) Ladder operators L_+ and L_- : Let us define the operators

$$L_+ = L_x + iL_y \text{ and } L_- = L_x - iL_y \qquad ...(2)$$

Commutation Relations of L_z with L_+ and L_-

$$\begin{aligned}
[L_z, L_+] &= [L_z, L_x + iL_y] = [L_z, L_x] + i\, [L_z, L_y] \\
&= i\hbar\ \ L_y + i\, (-i\hbar\, L_x) \\
&= i\hbar\, L_y + \hbar\, L_x \\
&= \hbar\, [L_x + iL_y] = \hbar\, L_+ \qquad ...(3)
\end{aligned}$$

and

$$\begin{aligned}
[L_z, L_-] &= [L_z, L_x - iL_y] \\
&= [L_z, L_x] - i\, [L_z, L_y] \\
&= i\hbar\, L_y - i\, (-\, i\hbar\, L_x) \\
&= i\hbar\, L_y - \hbar\, L_x = -\, \hbar\, (L_x - i\, L_y) \\
&= -\, \hbar\, L_- \qquad ...(4)
\end{aligned}$$

$\therefore$ $[L_z, L_\pm] = \pm\, \hbar\, L_\pm$ ...(5)

Commutation Relation of L_+ and L_- mutually

$$\begin{aligned}
[L_+, L_-] &= [(L_x + iL_y), (L_x - iL_y)] \\
&= [L_x, L_x] - i\, [L_x, L_y] + i\, [L_y, L_x] + [L_y, L_y] \\
&= 0 - i\, (i\hbar\, L_z) + i\, (-\, i\hbar\, L_z) + 0 \\
&= \hbar\, L_z + \hbar\, L_z \qquad ...(6)
\end{aligned}$$

$[L_+, L_-]$ $= 2\, \hbar\, L_z.$

(f) Commutation relation of orbital angular momentum with position

$$[L_x, x] = [L_x x - xL_x]$$

$$= \left\{y\left(-i\hbar\frac{\partial}{\partial z}\right) - z\left(-i\hbar\frac{\partial}{\partial y}\right)\right\}x - x\left\{y\left(-i\hbar\frac{\partial}{\partial z}\right) - z\left(-i\hbar\frac{\partial}{\partial y}\right)\right\}$$

If $\psi(x)$ is a function of x, we have

$$(L_x x - xL_x)\,\psi = \left\{y\left(-i\hbar\frac{\partial}{\partial z}(x\psi)\right) - z\left(-i\hbar\frac{\partial}{\partial y}(x\psi)\right)\right\} - x\left\{y\left(-i\hbar\frac{\partial\psi}{\partial z}\right) - z\left(-i\hbar\frac{\partial\psi}{\partial y}\right)\right\}$$

$$= 0$$

or $\quad [L_x, x] = 0$

Similarly,

$$[L_x, y] = i\hbar z; \quad [L_x, z] = -i\hbar y;$$
$$[L_y, y] = 0; \quad [L_y, z] = i\hbar x; \; [L_y, x] = -i\hbar z, \quad ...(7)$$
$$[L_z, y] = -i\hbar x; \quad [L_z, z] = 0; \; [L_z, x] = i\hbar y$$

Similarly, relations between **L** and **p** vectors by keeping in mind the cyclic order of the indices are

$$x \to y,\; y \to z,\; z \to x.$$

Thus $\quad [L_x, p_x] = 0,\; [L_x, p_y] = i\hbar p_z,\; [L_x, p_z] = -i\hbar p_y$ etc.

4.2.4. Hermitian operator

Definition. An operator A operating on any two functions $\psi_m(x)$ and $\psi_n(x)$ is said to be *Hermitian*, if it satisfies the relation

$$\int \psi_m^* A\psi_n \, dx = \int (A^*\psi_m^*)\psi_n \, dx \quad ...(1)$$

The integration here is over the domain in which the functions $\psi_m(x)$ and $\psi_n(x)$ are defined.

If an operator satisfies Eq. (1) whenever $\psi_m(x)$ and $\psi_n(x)$ are normalisable, we call it Hermitian, or self-adjoint.

Properties of Hermitian Operators

1. *The eigenvalues of Hermitian operators are real.*

Proof. Consider the eigenvalue equation of a Hermitian operator A such that

$$A\psi_n(x) = a_n\psi_n(x) \quad ...(1)$$

Multiplying Eq. (1) from left by ψ_n^* and integrating with respect to x from $-\infty$ to $+\infty$, we have

$$\int_{-\infty}^{\infty} \psi_n^* A\psi_n dx = a_n\int_{-\infty}^{\infty} \psi_n^*\psi_n \, dx = a_n \quad ...(2)$$

When the Hermitian property of A is used, Eq. (2) reduces to

$$\int_{-\infty}^{\infty} (A^*\psi_n^*)\psi_n \, dx = a_n$$

or $\quad a_n^*\int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx = a_n$

$$\therefore \quad a_n^* = a_n \quad ...(3)$$

Eq. (3) is possible only if a_n is real.

This proves that *the eigen values of a Hermitian operator are real.*

2. *Eigenfunctions of a Hermitian operator that belong to distinct eigenvalues are orthogonal.*

Proof: Let the Hermitian operator be A.

Let the eigen functions be $\psi_n(x)$, $\psi_m(x)$ with corresponding eigen values a_n, a_m. That is

$$A\,\psi_n(x) = a_n\,\psi_n(x) \qquad ...(1)$$

and

$$A\,\psi_m(x) = a_m\,\psi_m(x) \qquad ...(2)$$

Multiplying Eq. (1) from left by ψ^*_m and integrating in the limits $-\infty$ to $+\infty$, we get

$$\int_{-\infty}^{\infty} \psi_m^* A\psi_n\,dx = a_n \int_{-\infty}^{\infty} \psi_m^* \psi_n\,dx$$

Since operator A is Hermitian,

$$\int_{-\infty}^{\infty} A^* \psi_m^* \psi_n\,dx = a_n \int_{-\infty}^{\infty} \psi_m^* \psi_n\,dx$$

or

$$a_m \int_{-\infty}^{\infty} \psi_m^* \psi_n\,dx = a_n \int_{-\infty}^{\infty} \psi_m^* \psi_n\,dx$$

or

$$(a_m - a_n)\int_{-\infty}^{\infty} \psi_m^* \psi_n\,dx = 0$$

Since the eigenvalues are distinct, $(a_m - a_n) \neq 0$.

$\therefore$

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n\,dx = 0 \qquad ...(3)$$

That is, ψ_m and ψ_n are orthogonal.

Example. *Show that the momentum operator* $\frac{\hbar}{i}\cdot\frac{\partial}{\partial x}$ *is Hermitian.* (*Purvanchal 2005*)

Sol. Momentum operator $\hat{p} = \frac{\hbar}{i}\cdot\frac{\partial}{\partial x}$

Complex conjugate of $\hat{p}$, $\hat{p}* = -\frac{\hbar}{i}\cdot\frac{\partial}{\partial x}$

If $\hat{p}$ is hermitian operator, then in a given state ψ, its average value should be real.

i.e, $\langle\hat{p}\rangle = \int_{-\infty}^{\infty} \psi * \frac{\hbar}{i}\cdot\frac{\partial\psi}{\partial x}dx$ should be real.

Integrating the equation by parts,

$$\langle\hat{p}\rangle = \frac{\hbar}{i}[\psi * \psi]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\hbar}{i}.\frac{\partial\psi *}{\partial x}\psi\,dx = \int_{-\infty}^{\infty} \psi\left(-\frac{\hbar}{i}\cdot\frac{\partial\psi *}{\partial x}\right)dx = \langle p*\rangle$$

Since the expectation value of $\hat{p}$ is equal to the expectation value of its complex conjugate $\hat{p}*$, it is obvious that $\langle\hat{p}\rangle$ is real. Hence the momentum operator $\hat{p}$ is hermitian.

II Method. *Prove that the operator* $-i\hbar\frac{d}{dx}$ *is Hermitian.*

Sol. Consider the integral

$$\int_{-\infty}^{\infty} \psi_a^* \left(-i\hbar\frac{d}{dx}\right)\psi_b\,dx \qquad ...(1)$$

I use integration by parts.

$$\int_{-\infty}^{\infty} \psi_a^* \left(-i\hbar \frac{d}{dx}\right) \psi_b \, dx = -i\hbar \left[\psi_a^* \psi_b \right]_{-\infty}^{\infty} + i\hbar \int_{-\infty}^{\infty} \psi_b \frac{d}{dx} \psi_a^* \, dx$$

I throw away the boundary term (first term on the R.H.S.) for the usual reason: ψ_a and ψ_b must go to zero at $\pm\infty$.

$$\therefore \quad \int_{-\infty}^{\infty} \psi_a^* \left(-i\hbar \frac{d}{dx}\right) \psi_b \, dx = \int_{-\infty}^{\infty} \left(-i\hbar \frac{d\psi_a}{dx}\right)^* \psi_b \, dx \qquad ...(2)$$

Eq. (2) is the condition for the operator $-i\hbar \frac{d}{dx}$ to be Hermitian. Hence, the operator $-i\hbar \frac{d}{dx}$ is Hermitian.

4.2.5. Parity Operator

For functions of the variable x, the parity operator $\hat{\pi}$ is defined as

$$\hat{\pi}\psi(x) = \psi(-x)$$

i.e., when the wavefunction $\psi(x)$ is operated by the parity operator, it gets reflected in its coordinates.

Properties of the Parity Operator

1. π-operator is a linear operator. Let the parity operator operate on wavefunctions ψ_1 and ψ_2. Then

$$\hat{\pi}[\psi_1(x) + \psi_2(x)] = \psi_1(-x) + \psi_2(-x) = \hat{\pi}\psi_1(x) + \hat{\pi}\psi_2(x)$$

Also, $$\hat{\pi}C\psi_1(x) = C\psi(-x) = C\,\hat{\pi}\psi(x).$$

Hence $\hat{\pi}$ operator is a linear operator.

2. $\hat{\pi}$ operator is Hermitian. The scalar product of two functions ψ and ϕ is defined as

$$(\phi, \psi) = (\psi, \phi)^* = \int \phi^* \psi \, dx \qquad ...(1)$$

Consider the scalar product of $\hat{\pi}\psi$ and a function ϕ *i.e.*,

$$(\hat{\pi}\psi, \phi) = \int_{-\infty}^{+\infty} \psi^*(-x)\, \phi(x)\, dx = \int_{-\infty}^{+\infty} \psi^*(x')\, \phi(-x')\, dx'$$

The second integral is obtained from the first by the substitution $x' = -x$.

Since the value of the integral is unaffected by renaming the variable of integration, we have

$$(\hat{\pi}\psi, \phi) = \int_{-\infty}^{\infty} \psi^*(x)\, \phi(-x)\, dx = (\psi, \hat{\pi}\phi) \qquad ...(2)$$

Eq. (2) shows that $\hat{\pi}$ is a Hermitian operator.

The eigenvalues of $\hat{\pi}$ are therefore real.

3. Eigenvalues of parity operator. The eigenvalue of the $\hat{\pi}$ operator is given by

$$\hat{\pi}\psi = \lambda\psi. \qquad ...(1)$$

Here, λ is the eigenvalue of the operator $\hat{\pi}$.

Operating Eq. (1) again by $\hat{\pi}$ operator, we have

$$\hat{\pi}^2\psi = \hat{\pi}(\lambda\psi) = \lambda(\hat{\pi}\psi) = \lambda(\lambda\psi) = \lambda^2\psi \qquad ...(2)$$

From definition of parity operator

$$\hat{\pi}\psi(x) = \psi(-x)$$

$$\hat{\pi}[\hat{\pi}\,\psi(x)] = \hat{\pi}\,\psi(-x) = \psi(x)$$

$$\hat{\pi}^2\psi(x) = \psi(x) \qquad ...(3)$$

Comparing Eqs. (2) and (3), we note that the eigen values of π-operator satisfy the equation

$$\lambda^2 = 1$$

or $$\lambda = \pm 1. \qquad ...(4)$$

The eigenfunctions corresponding to eigenvalue $\lambda = +1$ of the parity operator are the even functions ψ_e, which satisfy

$$\psi_e(x) = \psi_e(-x). \qquad ...(5)$$

The odd functions ψ_o belong to the eigenvalue $\lambda = -1$ and satisfy the relation

$$\psi_o(x) = -\psi_o(-x). \qquad ...(6)$$

The eigenfunctions of $\hat{\pi}$ are a complete set with respect to the class of functions of x. This is shown by the identity

$$\psi(x) = \frac{1}{2}[\psi(x)+\psi(-x)] + \frac{1}{2}[\psi(x)-\psi(-x)] \qquad ...(7)$$

Thus any $\psi(x)$ is a linear combination of an *even* function of x, $[\psi(x) + \psi(-x)]$, and an *odd* function of x, $[\psi(x) - \psi(-x)]$.

- The parity operation in three dimensions is de ined by re lecting all three axes according to the coordinate transformation $(x, y, z) \rightarrow (-x, -y, -z)$ [Fig. 4.2].

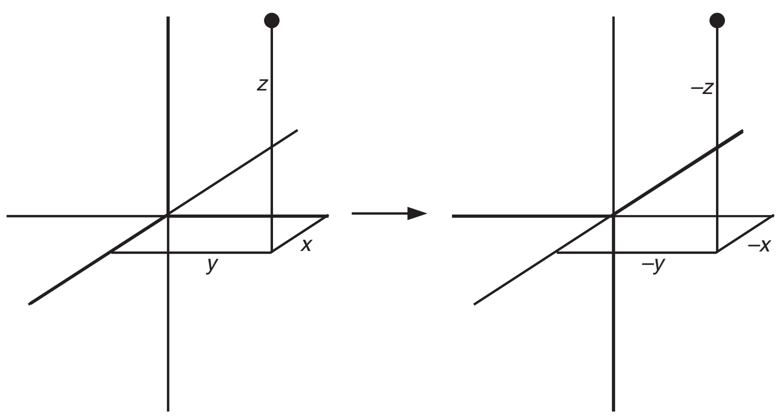


Fig. 4.2

The operation is also called *space inversion* as the transformation changes a right-handed system of coordinates into a left handed system.

The Parity operator $\hat{\pi}$ is defined by the relation

$$\hat{\pi}\,\psi(\mathbf{r}) = \psi(-\mathbf{r}).$$

Thus the parity operator corresponds to an inversion of the position coordinate **r** through the origin.

4.2.6 Probability Density

Let $\psi(x, t)$ be a normalised wave function of a particle in a given state. $\psi(x, t)$ by itself is sometimes called *Probability amplitude* for the position of the particle.

The product $\psi^*(x, t)\,\psi(x, t)$ is called *probability density* and is real and hence observable. It is the probability of finding the particle in unit interval of space centered about x at time t.

Probability density = $\psi^* (x, t)\, \psi (x, t) = |\psi (x, t)|^2$ …(1)

A large value of $|\psi|^2$ means the strong possibility of the particle's presence. A small value of $|\psi|^2$ means the slight possibility of the particle's presence. This interpretation was made by Max Born.

The probability that the particle may be found in the region between x and $(x + dx)$ at time t is

$$P = \psi^* (x, t)\, \psi (x, t)\, dx \quad ...(2)$$

The probability of finding the particle in a volume element $d\tau = dx\, dy\, dz$ about any point **r** at time t is expressed as

$$P(\mathbf{r}, t)\, d\tau = |\psi(\mathbf{r}, t)|^2\, d\tau. \quad ...(3)\backslash$$

4.2.7. Probability Current Density

Suppose $\psi(\boldsymbol{r}, t)$ is the state function representing a one-particle system.

The probability that the particle is in the finite volume τ is

$$P = \int_\tau \psi^* \psi\, d\tau \quad ...(1)$$

The rate of change of this probability is

$$\frac{dP}{dt} = \int_\tau \left(\psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t} \right) d\tau \quad ...(2)$$

Time-dependent Schrodinger equation is

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

Assuming V to be real, complex conjugate of Eq. (3) is

$$-\frac{\hbar^2}{2m}\nabla^2 \psi^* + V\psi^* = -i\hbar \frac{\partial \psi^*}{\partial t} \quad ...(4)$$

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

$$\therefore \quad \psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t} = -\frac{i\hbar}{2m}\left[\psi \nabla^2 \psi^* - \psi^* \nabla^2 \psi \right]$$

$$= -\frac{i\hbar}{2m}\nabla.\left(\psi \nabla \psi^* - \psi^* \nabla \psi \right)$$

We define probability current density as

$$\mathbf{j} = \frac{i\hbar}{2m}\left[\psi \nabla \psi^* - \psi^* \nabla \psi \right] \quad ...(5)$$

$$\therefore \int_\tau \left(\psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t} \right) d\tau = -\int_\tau \nabla.\mathbf{j}\, d\tau$$

Eq. (2) becomes $$\frac{dP}{dt} = -\int_\tau \nabla.\mathbf{j}\, d\tau \quad ...(6)$$

The volume integral can be transformed to a surface integral by Gauss's theorem, *i.e.*,

$$\frac{dP}{dt} = -\oint_S \mathbf{j}.d\mathbf{S} \quad ...(7)$$

Here S is the surface enclosing the volume τ. The direction of $d\boldsymbol{S}$ is along the outward normal. Clearly from Eq. (7), the integral of $\boldsymbol{j}$ over the surface S is the probability that the particle will cross the surface going outwards in unit time.

From Eqs. (2) and (6), $\frac{\partial}{\partial t}(\psi^* \psi) + \nabla.\boldsymbol{j} = 0$ ...(8)

This equation expresses the *conservation of probability density*. It is analogous to the equations of continuity of hydrodynamics and electrodynamics.

4.3. DERIVATION OF TIME-DEPENDENT FORM OF SCHRÖDINGER 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

$$\psi = Ae^{-i\omega(t - x/v)} \quad ...(1)$$

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

$$\therefore \quad \psi = Ae^{-2\pi i(\nu t - x/\lambda)} \quad ...(2)$$

Let E be the total energy and p the momentum of the particle.

Then, $\nu = \frac{E}{h}$ and $\lambda = \frac{h}{p}$.

Making these substitutions in Eq. (2),

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

$$\psi = Ae^{-(i/\hbar)(Et - px)} \quad ...(3)$$

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

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

$$p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2} \quad ...(4)$$

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

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

$$E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t} \quad ...(5)$$

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.

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

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

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

Substituting the expressions for $E\psi$ and $p^2\psi$ from Eqs. (5) and (4) into Eq. (7), we obtain

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

or

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \quad ...(8)$$

Eq. (8) is the *time-dependent form of Schrödinger's equation in one dimension.*

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

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + V\psi.$$

Here, the particle's potential energy V is some function of x, y, z, and t.

Schrödinger's equation : Steady-state form — Time independent Schrödinger equation

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, Schrödinger'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

$$\psi = Ae^{-(i/\hbar)(Et-px)} = Ae^{-(iE/\hbar)t}.e^{+(ip/\hbar)x}$$

$$\therefore \qquad \psi = \psi_0 \, e^{-(iE/\hbar)t} \qquad ...(1)$$

Here, $\psi_0 = Ae^{+(ip/\hbar)x}$. That is, ψ is the product of a position dependent function ψ_0 and a time-dependent function $e^{-(iE/\hbar)t}$.

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

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\psi_0 \, e^{-(iE/\hbar)t} \qquad ...(2)$$

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

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial^2 \psi_0}{\partial x^2} e^{-(iE/\hbar)t} \qquad ...(3)$$

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

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

$$\therefore \qquad E\psi_0 \, e^{-(iE/\hbar)t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi_0}{\partial x^2} e^{-(iE/\hbar)t} + \mathrm{V}\psi_0 \, e^{-(iE/\hbar)t}$$

Dividing through by the common exponential factor, we get

$$\frac{\partial^2 \psi_0}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\,\psi_0 = 0 \qquad ...(4)$$

Eq. (4) is the *steady-state form of Schrödinger's equation.*

In three dimensions, it is

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

Usually it is written in the form

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

Steady-state form of Schrödinger's equation in three dimensions is

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

Eigenvalues and Eigenfunctions

The values of energy E_n for which Schrödinger's steady-state equation can be solved are called **eigenvalues**. The corresponding wave functions ψ_n are called **eigenfunctions**.

Degeneracy. If there is more than one linearly independent wave function belonging to the same energy eigenvalue E, the energy level is said to be degenerate. If there are g linearly independent wave functions (ψ_1, ψ_2, ... ψ_g) belonging to the same energy state, then the energy level is said to be g-fold degenerate.

The degree of degeneracy is defined as the number of linearly independent eigen functions corresponding to the same eigen value.

Operator for Momentum

The wave function for a free particle moving in the positive x-direction is

$$\psi(x, t) = Ae^{i/\hbar(p_x x - Et)} \quad ...(1)$$

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

$$\frac{\partial\psi}{\partial x} = A\left(\frac{i}{\hbar}\right) p_x \, e^{i/\hbar(p_x x - Et)} = \frac{i}{\hbar} p_x \, \psi$$

or

$$\frac{\hbar}{i}\frac{\partial\psi}{\partial x} = p_x \, \psi$$

$\therefore$

$$-i\hbar\frac{\partial}{\partial x}\psi = p_x \, \psi \quad ...(2)$$

Evidently the dynamical quantity p_x in some sense corresponds to the differential operator $-i\hbar\frac{\partial}{\partial x}$.

We denote operators by using a caret.

$\hat{p}_x$ is the operator that corresponds to x-component of the momentum p_x.

From Eq. (2), for the x-component of the momentum, the operator is

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \quad ...(3)$$

The **operator representation** of $\boldsymbol{p}$ is

$$\hat{\boldsymbol{p}} = -i\hbar\nabla \quad ...(4)$$

To obtain the expectation value of the momentum p_x

The expectation value of p_x is found by using the corresponding differential operator.

$$\langle p_x \rangle = \int_{-\infty}^{+\infty} \psi^*(x, t)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x, t)\, dx$$

8.1.1. Properties of the Wave Function

Physical significance of ψ

- By applying Schrödinger's equation to the motion of a particle, we get the wave function ψ. The future course of the particle's motion—like its initial state—is a matter of probabilities instead of certainties.
- The quantity whose variations make up matter waves is called the **wave function,** Ψ. This function can be either real or complex.

  The wave function Ψ itself, however, has no direct physical significance.
- The only quantity having a physical meaning is the square of its magnitude $P = |\psi|^2 = \psi\psi^*$.

  Here, ψ^* is the complex conjugate of ψ.

  The quantity P is the probability density.
- $|\Psi|^2$, the square of the absolute value of the wave function, is called **probability density**.

  The probability of experimentally finding the body described by the wave function Ψ at the point x, y, z at the time t is proportional to the value of $|\Psi|^2$ there at t.

  A large value of $|\Psi|^2$ means the strong possibility of the body's presence.

A small value of $|\Psi|^2$ means the slight possibility of its presence.

This interpretation was made by Max Born.

- The probability of finding a particle in a volume *dx dy dz* is $|\psi|^2\, dx\, dy\, dz$.
- The particle is certainly to be found somewhere in space.

$$\therefore \quad \iiint |\psi|^2\, dx \,.\, dy \,.\, dz = 1.$$

The triple integral extends over all possible values of *x, y, z*.

A wave function (ψ) satisfying this relation is called a *normalised wave function.*

Orthogonal wave function

If the product of a function $\psi_1(x)$ and the complex conjugate $\psi_2^*(x)$ of a function $\psi_2(x)$ vanishes when integrated with respect to *x* over the interval $a \le x \le b$, that is, if

$$\int_a^b \psi_2^*(x)\, \psi_1(x)\, dx = 0,$$

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

Normalised wave function

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 unity, *i.e.*,

$$\int \psi\psi^*\, dV = \int |\psi|^2\, dV = 1.$$

Here, the integration extends over all space.

Any wave function satisfying the above equation is said to be 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
$$|A|^2 = \frac{1}{\int \psi\psi^*\, dx\, dy\, dz}$$

$|A|$ is called normalizing constant.

Orthonormal functions. The functions which are orthogonal and also normalised are called orthonormal functions.

Requirements of wave function

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 Schrödinger 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 $x \to \pm\infty$

UNIT V

APPLICATIONS OF SCHRÖDINGER EQUATION

Particle in a one-dimensional box – Particle in a rectangular three-dimensional box. Simple harmonic oscillator – One dimensional simple harmonic oscillator in quantum mechanics – zero-point energy. Reflection at step potential – Transmission across a potential barrier – Barrier Penetration (tunnelling effect).

APPLICATIONS OF SCHRÖDINGER'S EQUATION

5.1 THE FREE PARTICLE

A free particle is defined as one which is subject to no forces of any kind, and so, moves in a region of constant potential. The particle motion is confined to the x-axis only. We shall consider the potential to be zero, $V = 0$.

The time-independent Schrödinger equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad ...(1)$$

Define a quantity k, called the wave number, by

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad ...(2)$$

$$\therefore \quad \frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad ...(3)$$

The solution of Eq. (3) is

$$\psi = A\,e^{ikx} + B\,e^{-ikx} \qquad ...(4)$$

Let us set $B = 0$. Then

$$\psi = A\,e^{ikx} \qquad ...(5)$$

Eq. (5) describes a particle moving in the positive x-direction.

A problem appears in normalising the wave function. We ought to have

$$\int_{-\infty}^{\infty} \psi^*\psi\,dx = A^2\int_{-\infty}^{\infty} dx = 1 \qquad ...(6)$$

$\int_{-\infty}^{\infty} dx$ is infinite. So A must be zero. This difficulty arises since we are considering an ideal case of infinite length. In practice, the particle is confined to a finite length so that normalisation is possible.

The probability density for the particle is $\psi^*\psi = A^2$, a constant independent of x. Consequently, the particle is equally likely to be found anywhere. So we have an infinite amount of uncertainty in its position, *i.e.*, $\Delta x = \infty$. According to the expression $\Delta p\,\Delta x \geq \hbar/2$, Δp must be zero.

Let us prove this.

$$< p > = \int_{-\infty}^{\infty} \psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi\,dx = \hbar k\int_{-\infty}^{\infty} \psi*\psi\,dx = \hbar k$$

Notice that $< p >$ is positive, meaning that our particle has a momentum of exactly $\hbar k$ and is moving toward the right.

$$< p^2 > = \int_{-\infty}^{\infty} \psi^*\left(-\hbar^2\right)\frac{\partial^2}{\partial x^2}\psi\,dx = -\hbar^2\left(-k^2\right)\int_{-\infty}^{\infty} \psi^*\psi\,dx$$

$$= \hbar^2 k^2$$

$$\therefore \quad (\Delta p)^2 = < p^2 > - < p >^2 = 0\,.$$

Thus the momentum of the particle is precisely defined.

Note that for the particle in a square well, the energy is quantised. But for the free particle, there is no such restriction on the energy. Generally, bound systems (such as electrons trapped in an atom) will give rise to discrete energy levels. Unbound systems (such as two atoms that collide) will give rise to an energy continuum.

5.2 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. 5.1). 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

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

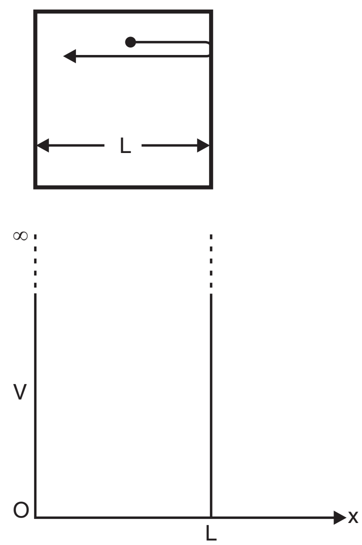


Fig. 5.1

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

Within the box, the Schrödinger's equation becomes

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

The general solution of this equation is

$$\psi = A \sin \frac{\sqrt{2mE}}{\hbar} x + B \cos \frac{\sqrt{2mE}}{\hbar} x \qquad ...(2)$$

A and B are constants to be evaluated.

The boundary conditions are used to evaluate the constants A and B in Eq. (2).

(*i*) $\psi = 0$ at $x = 0$. Hence $B = 0$.

(*ii*) $\psi = 0$ at $x = L$.

ψ will be 0 at $x = L$ only when

$$\frac{\sqrt{2mE}}{\hbar} L = n\pi \qquad n = 1, 2, 3, ... \qquad ...(3)$$

From Eq. (3) it is clear that the energy of the particle can have only certain values, which are the eigen values.

These eigenvalues are found by solving Eq. (3) for E_n.

$$\therefore \qquad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, 3, ... \qquad ...(4)$$

For each value of n, there is an energy level. Each value of E_n is called an *eigenvalue.* Thus inside the box, the particle can only have the *discrete* energy values specified by Eq. (2). Note also that the particle cannot have zero energy.

Wave Functions

The wave functions of a particle in a box whose energies are E_n are, from Eq. (2) with $B = 0$.

$$\psi_n = A \sin \frac{\sqrt{2mE_n}}{\hbar} x \qquad ...(5)$$

Substituting Eq. (4) for E_n gives

$$\psi_n = A \sin \frac{n\pi x}{L} \quad ...(6)$$

ψ_n are the eigenfunctions corresponding to the energy eigenvalues E_n.

Evaluation of *A* and Normalization of the Wave Function

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

$$\int_0^L \psi^* \psi \, dx = 1 \text{ i.e., } A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

i.e., $$A^2 \int_0^L \left(\frac{1-\cos 2n\pi x/L}{2}\right) dx = 1 \quad \text{or } A^2 \frac{L}{2} = 1$$

or $$A = \sqrt{\frac{2}{L}}$$

The normalized wave functions of the particle are

$$\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \qquad n = 1, 2, 3, ... \quad ...(7)$$

The normalised wave functions ψ_1, ψ_2, and ψ_3 together with the probability densities $|\psi_1|^2$, $|\psi_2|^2$, and $|\psi_3|^2$ are plotted in Fig. 5.2.

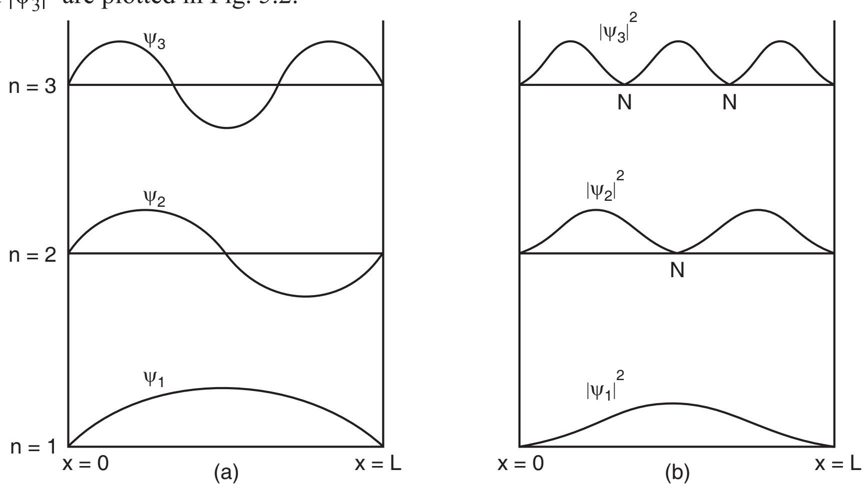


Fig. 5.2

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

Sol. Here, m = mass of the electron = 9.1×10^{-31} kg; $L = 1$Å $= 10^{-10}$ m, $E_n = ?$

$\therefore$ The permitted electron energies = $E_n = \dfrac{n^2\pi^2\hbar^2}{2mL^2}$

$$E_n = \frac{n^2\pi^2 (1.054 \times 10^{-34})^2}{2(9.1 \times 10^{-31})(10^{-10})^2} = 6 \times 10^{-18}\, n^2\, J = 38n^2\, eV.$$

The minimum energy, the electron can have, is $E_1 = 38\, eV$, corresponding to $n = 1$.

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

EXAMPLE 2. *Calculate the expectation value $<p_x>$ of the momentum of a particle trapped in a one-dimensional box.*

SOL. The normalized wave functions of the particle are

$$\psi_n^* = \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$\frac{d\psi}{dx} = \sqrt{\frac{2}{L}} \left(\frac{n\pi}{L}\right) \cos \frac{n\pi x}{L}$$

Now,
$$<p_x> = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{d}{dx}\right) \psi \, dx$$

$$= -i\hbar \frac{2}{L} \frac{n\pi}{L} \int_0^L \sin \frac{n\pi x}{L} \cos \frac{n\pi x}{L} \, dx$$

$$= 0$$

The expectation value $<p_x>$ of the particle's momentum is 0.

EXAMPLE 3. *Find the expectation value $<x>$ of the position of a particle trapped in a box L wide.*

SOL.
$$< x > = \int_{-\infty}^{\infty} x \, |\psi|^2 \, dx = \frac{2}{L} \int_0^L x \sin^2 \frac{n\pi x}{L} \, dx$$

$$= \frac{2}{L} \left[\frac{x^2}{4} - \frac{x \sin(2n\pi x/L)}{4n\pi/L} - \frac{\cos(2n\pi x/L)}{8(n\pi/L)^2} \right]_0^L$$

$$\therefore \quad < x > = \frac{2}{L}\left(\frac{L^2}{4}\right) = \frac{L}{2}.$$

This result means that the average position of the particle is the middle of the box in all quantum states.

EXAMPLE 4. *Verify the orthogonal property of wave functions of a particle in a one dimensional box.*

SOL. The wave functions of a particle in one dimensional box are

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

We want to verify

$$\int_0^L \psi_n^*(x) \psi_m(x) dx = 0 \text{ for } n \neq m.$$

$$\text{L.H.S} = \int_0^L \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \sqrt{\frac{2}{L}} \sin \frac{m\pi x}{L} dx = \frac{1}{L} \int_0^L \left(2 \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L}\right) dx$$

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

$$\therefore \quad \text{L.H.S} = 0. \text{ Hence verified.}$$

5.3 FINITE SQUARE POTENTIAL WELL

Fig. 5.3 shows a square potential well of width L. Consider a particle with energy E moving along the x-axis. The energy E of the trapped particle is less than the height U of the barriers. Schrodinger's steady-state equation for regions I and III is

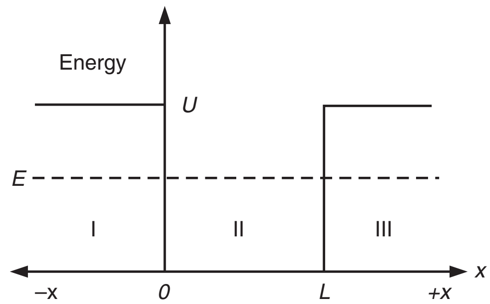


Fig. 5.3

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}(E-U)\psi = 0$$

Put $$\frac{\sqrt{2m(U-E)}}{\hbar} = a \qquad ...(1)$$

$$\frac{d^2\psi}{dx^2}-a^2\psi = 0 \quad x<0, x>L, \qquad ...(2)$$

The solutions to Eq. (2) are :

$$\psi_I = A\,e^{ax}+B\,e^{-ax} \qquad ...(3)$$

$$\psi_{III} = C\,e^{ax}+D\,e^{-ax} \qquad ...(4)$$

For ψ to remain finite as $x \to \pm\infty$, we must have $B = 0$ and $C = 0$.

$\therefore$ $$\psi_I = A\,e^{ax} \qquad ...(5)$$

$$\psi_{III} = D\,e^{-ax} \qquad ...(6)$$

These wave functions decrease exponentially inside the barriers at the sides of the well.

Schrödinger's equation for region II is

$$\frac{d^2\psi}{dx^2}+\frac{2mE}{\hbar^2}\psi = 0 \qquad ...(7)$$

The solution of Eq. (7) is

$$\psi_{II} = F\sin\frac{\sqrt{2mE}}{\hbar}x+G\cos\frac{\sqrt{2mE}}{\hbar}x \qquad ...(8)$$

At the boundaries $x = 0$ and $x = L$, the wave functions inside and outside must have the same value and the same slope.

$$\psi_{II} = \psi_I \text{ and } \frac{d\psi_{II}}{dx} = \frac{d\psi_I}{dx} \text{ at } x = 0.$$

$$\psi_{II} = \psi_{III} \text{ and } \frac{d\psi_{II}}{dx} = \frac{d\psi_{III}}{dx} \text{ at } x = L.$$

These conditions when applied to Eqs. (5), (6) and (8) yield the following relations :

$$G = A \qquad ...(9)$$

$$F\frac{\sqrt{2mE}}{\hbar} = Aa \qquad ...(10)$$

$$F\sin\frac{\sqrt{2mE}}{\hbar}L+G\cos\frac{\sqrt{2mE}}{\hbar}L = D\,e^{-aL} \qquad ...(11)$$

$$F\frac{\sqrt{2mE}}{\hbar}\cos\left(\frac{\sqrt{2mE}}{\hbar}L\right)-G\frac{\sqrt{2mE}}{\hbar}\sin\left(\frac{\sqrt{2mE}}{\hbar}L\right)=-Da\,e^{-aL} \quad ...(12)$$

Eqs. (9) and (10) give

$$F = Ga\frac{\hbar}{\sqrt{2mE}} \quad ...(13)$$

Eq. (13) together with Eqs. (11) and (12) yields

$$\tan\left(\frac{\sqrt{2mE}}{\hbar}L\right) = \frac{2a(\sqrt{2mE}/\hbar)}{\left(\frac{2mE}{\hbar^2}-a^2\right)}$$

$$\therefore \quad \tan\left(\frac{\sqrt{2mE}}{\hbar}L\right) = \frac{2\sqrt{E(U-E)}}{2E-U} \quad ...(14)$$

Only those values of E which satisfy this relation are the allowed energy states. Thus the energy is quantised. The allowed energy values are found by numerical or graphical methods.

The wave functions for the first three allowed energy values and the corresponding probability densities for finding the particle at different locations are shown in Figure 5.4 (*a*) and (*b*) respectively. The particle has a certain probability of being found outside the wall.

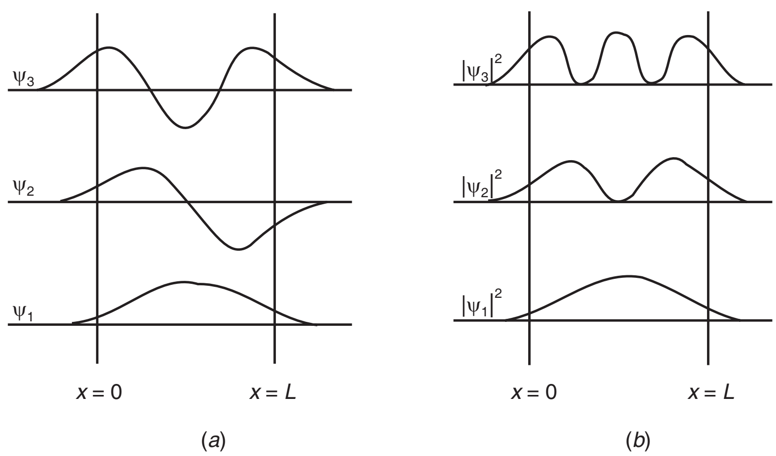


Fig. 5.4

5.4 RECTANGULAR POTENTIAL WELL

A one dimensional rectangular potential well is defined by

$$V(x) = \begin{cases} 0 & (x<0), \\ -V_0 & (0<x<a), \\ 0 & (x>a), \end{cases} \quad ...(1)$$

V_0 , the *depth of the well*, is a positive number (Fig. 5.5). When total energy of the particle is negative ($-V_0 < E < 0$), the particle is confined to the well and forms bound states. m is the mass of the particle.

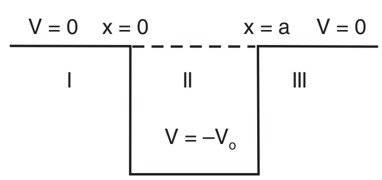


Fig. 5.5

The Schrödinger equation for the three regions are

$$\frac{d^2\psi_1}{dx^2}+\frac{2mE}{\hbar^2}\psi_1 = 0 \text{ or } \frac{d^2\psi_1}{dx^2}-\lambda^2\psi_1 = 0 \quad (x<0)$$

$$\frac{d^2\psi_2}{dx^2}+\frac{2m(E+V_0)}{\hbar^2}\psi_2 = 0 \text{ or } \frac{d^2\psi_2}{dx^2}+k^2\psi_2 = 0 \quad (0<x<a)$$

$$\frac{d^2\psi_3}{dx^2}+\frac{2mE}{\hbar^2}\psi_3 = 0 \text{ or } \frac{d^2\psi_3}{dx^2}-\lambda^2\psi_3 = 0 \quad (x>a)$$

Here, $\lambda = \sqrt{\frac{-2mE}{\hbar^2}}$ and $k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$

The solutions of the Schrödinger equation outside the potential well are now $e^{\lambda x}$ and $e^{-\lambda x}$. Here λ is real. When $x \to \infty$, $e^{\lambda x}$ is not bounded. Hence it must not appear in ψ for $x > a$. Similarly, ψ must not contain $e^{-\lambda x}$ for $x < 0$.

The (unnormalised) wave functions are

$$\psi_1 = e^{\lambda x} \qquad (x<0),$$
$$\psi_2 = A\,e^{ikx} + B\,e^{-ikx} \qquad (0<x<a)$$
$$\psi_3 = C\,e^{-\lambda x} \qquad (x>a) \qquad ...(2)$$

The continuity of ψ and $d\psi/dx$ *at* $x = 0$ and $x = a$ require that

$$\psi_1 = \psi_2 \text{ at } x = 0$$
$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \text{ at } x = 0$$
$$\psi_2 = \psi_3 \text{ at } x = a$$
$$\frac{d\psi_2}{dx} = \frac{d\psi_3}{dx} \text{ at } x = a\cdot$$

These conditions give four relations between the three constants A, B, C.

$$1 = A + B$$
$$\lambda = ik(A-B)$$
$$C\,e^{-\lambda a} = A\,e^{ika} + B\,e^{-ika}$$
$$-\lambda\; C\,e^{-\lambda a} = ik(A\,e^{ika} - B\,e^{-ika}) \qquad ...(3)$$

These equations will give a unique solution, only if

$$2\cot ka = \frac{k}{\lambda}-\frac{\lambda}{k} \qquad ...(4)$$

This is a transcendental equation in k.

If this condition is satisfied, the solution is

$$A = B^* = \frac{1}{2}\left(1-i\frac{\lambda}{k}\right), C = \frac{1}{2}\left(\frac{k}{\lambda}+\frac{\lambda}{k}\right)e^{\lambda a}\sin ka \qquad ...(5)$$

To solve Eq. (4) graphically, introduce the quantities

$$\gamma = \sqrt{\frac{2mV_0 a^2}{\hbar^2}}, \alpha = \frac{k\,a}{\gamma} = \sqrt{1+\frac{E}{V_0}} \qquad ...(6)$$

Then Eq. (4) can be expressed as

$$\gamma\,\alpha = (n-1)\,\pi + 2\cos^{-1}\alpha, \ (n = 1, 2, ...) \qquad ...(7)$$

Fig. 5.6 illustrates this relation graphically for the two cases $\gamma = 1, 4$. The abscissae of the points of intersection (denoted by dots) of the two graphs give the energies of the corresponding states according to the formula

$$E = -V_0\,(1-\alpha^2) \qquad ...(8)$$

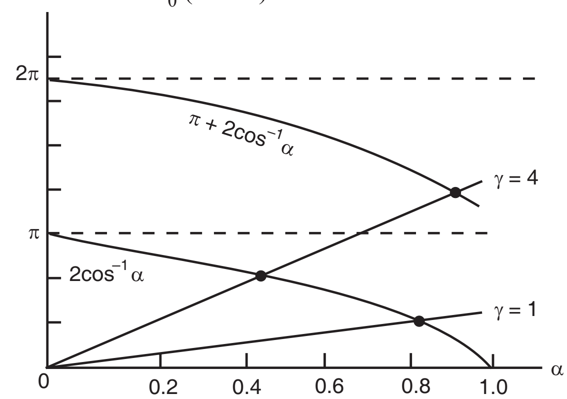


Fig. 5.6

The number of states for a given well depth is clearly the greatest integer contained in the quantity $(\gamma/\pi + 1)$. This quantity increases as V_0 is made larger. The values of E corresponding to the stationary states decreases as the well depth increases. A new level appears at zero energy each time γ assumes the value $n\,\pi$. Energy-level diagrams for the two cases of Fig. 5.6 are drawn in Fig. 5.7. n is the *quantum number* ranking the energy levels in increasing order.

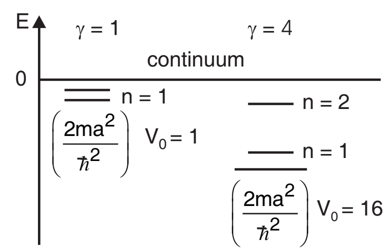


Fig. 5.7

Substituting the values of A, B and C from Eq. (5) in Eq. (2),

$$\psi_1 = e^{\lambda x} \qquad (x < 0),$$

$$\psi_2 = \frac{1}{\alpha}\sin\left[k\left(x-\frac{a}{2}\right)+\frac{n\pi}{2}\right] \qquad (0 < x < a),$$

$$\psi_3 = (-1)^{n+1}\,e^{-\lambda(x-a)} \qquad (x > a) \qquad ...(9)$$

ψ is zero at $x = \pm\infty$ and at $(n-1)$ points within the region $0 < x < a$. So the total number of zeros of ψ is $n + 1$. The wave function for $n = 5$ is shown in Fig. 5.8.

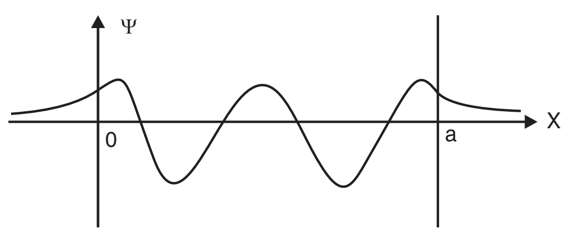


Fig. 5.8

For an *infinitely deep potential well*, the straight line of Fig. 8.6 approaches the vertical axis. The points of intersection approach the values

$$k\,a = n\,\pi \qquad (n = 1, 2, ...) \qquad ...(10)$$

Hence the energy levels are

$$\frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2m\,a^2} \qquad ...(11)$$

For $E > 0$, well behaved solutions can be obtained for all values of E. So the energy spectrum is a continuum in this case.

5.5 THE SQUARE WELL IN THREE DIMENSIONS

Consider a particle of mass *m* which is restricted to move in a box with sides *a*, *b* and *c* (Fig. 5.9). The potential function $V(x, y, z)$ is having a constant value of zero in the regions given as follows :

$$V(x, y, z) = 0, \qquad 0 < x < a,$$
$$V(x, y, z) = 0, \qquad 0 < y < b,$$
$$V(x, y, z) = 0, \qquad 0 < z < c.$$

The potential outside the box is infinite.

The Schrödinger time independent wave equation for the particle inside the box is given by

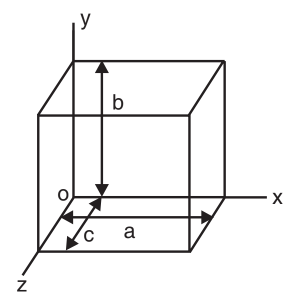


Fig. 5.9

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

Let us solve this equation by the method of separation of variables. Assume that the function ψ can be written as a product of three functions, *X*, *Y*, and *Z*. Each function depends on only one of the coordinates.

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

$$\frac{\partial^2 \psi}{\partial x^2} = X''\,Y\,Z, \frac{\partial^2 \psi}{\partial y^2} = X\,Y''\,Z, \frac{\partial^2 \psi}{\partial z^2} = X\,Y\,Z''.$$

Substituting this in Eq. (2) and dividing by *XYZ*, we get

$$\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} + \frac{2\,m\,E}{\hbar^2} = 0 \qquad ...(3)$$

We notice that each term of this equation depends on a different variable and that the three variables are independent. The last term is constant. The only way for the equation to remain valid for all values of *x*, *y*, and *z* in our interval is for *each* term of Eq. (3) to be constant. Therefore

$$\frac{X''}{X} = -\alpha^2,\ \frac{Y''}{Y} = -\beta^2,\ \frac{Z''}{Z} = -\gamma^2$$

where α, β and γ are constants. $\alpha^2 + \beta^2 + \gamma^2 = 2m\,E/\hbar^2$

These equations can be written as

$$\frac{d^2 X}{dx^2} + \alpha^2 X = 0 \qquad ...(4)$$

$$\frac{d^2 Y}{dy^2} + \beta^2 Y = 0 \qquad ...(5)$$

$$\frac{d^2 Z}{dz^2} + \gamma^2 Z = 0 \qquad ...(6)$$

The general solutions of (4), (5) and (6) are given by

$$X = A_1 \sin \alpha x + B_1 \cos \alpha x$$
$$Y = A_2 \sin \beta y + B_2 \cos \beta y$$
$$Z = A_3 \sin \gamma z + B_3 \cos \gamma z$$

Values of the constants $A_1, A_2, A_3, B_1, B_2, B_3$ can be found by applying boundary conditions. The boundary conditions require that the wave function vanishes at the box walls where the potential is infinite, *i.e.*,

$$\psi(0, y, z) = \psi(x, 0, z) = \psi(x, y, 0) = 0 \qquad ...(7)$$
$$\psi(a, y, z) = \psi(x, b, z) = \psi(x, y, c) = 0 \qquad ...(8)$$

Applying boundary conditions (7) to the above equations,

$$B_1 = B_2 = B_3 = 0$$

Applying boundary conditions (8) to the above equations

$$\sin \alpha a = 0, \text{ i. e., } \alpha a = n_x \pi \text{ or } \alpha = n_x\pi/a$$
$$\sin \beta b = 0, \text{ i. e., } \beta b = n_y \pi \text{ or } \beta = n_y\pi/b$$
$$\sin \gamma c = 0, \text{ i. e., } \gamma c = n_z \pi \text{ or } \gamma = n_z\pi/c$$

Here n_x, n_y, n_z are integers of which none is equal to zero.

$$\therefore \quad X = A_1 \sin \frac{n_x \pi x}{a} \qquad ...(9)$$
$$Y = A_2 \sin \frac{n_y \pi y}{b} \qquad ...(10)$$
$$Z = A_3 \sin \frac{n_z \pi z}{c} \qquad ...(11)$$

Substituting these values in Eq. (2), we get

$$\psi(x, y, z) = A_1 A_2 A_3 \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{b} \sin \frac{n_z \pi z}{c}$$
$$= A \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{b} \sin \frac{n_z \pi z}{c}$$

In the above equation A is the normalisation constant.

A can be found by using the normalisation condition

$$\int_0^a \int_0^b \int_0^c \psi \psi^* \, dx\, dy\, dz = 1 \qquad ...(12)$$

$$A^2 \int_0^a \int_0^b \int_0^c \sin^2 \frac{n_x \pi x}{a} \sin^2 \frac{n_y \pi y}{b} \sin^2 \frac{n_z \pi z}{c} \, dx\, dy\, dz = 1$$

$$\therefore \quad A^2 \frac{a}{2} \cdot \frac{b}{2} \cdot \frac{c}{2} = 1$$

or
$$A = \frac{2\sqrt{2}}{\sqrt{(abc)}} \qquad ...(13)$$

The normalised wave function is

$$\psi(x, y, z) = \frac{2\sqrt{2}}{\sqrt{(abc)}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{b} \sin \frac{n_z \pi z}{c} \qquad ...(14)$$

We have $\alpha^2 + \beta^2 + \gamma^2 = 2m\, E/\hbar^2$

$$\frac{n_x^2\,\pi^2}{a^2} + \frac{n_y^2\,\pi^2}{b^2} + \frac{n_z^2\,\pi^2}{c^2} = \frac{2\,m\,E}{\hbar^2}$$

$$\therefore \qquad E_{n_x n_y n_z} = \frac{\hbar^2\,\pi^2}{2\,m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c}\right] \qquad \text{...(15)}$$

Let us examine the case in which the particle is confined in a cubical region. Then $a = b = c$. The energy levels of Eq. (15) become

$$E_{\text{cube}} = \frac{\hbar^2\,\pi^2}{2\,m\,a^2}(n_x^2 + n_y^2 + n_z^2) \qquad \text{...(16)}$$

The *ground state energy* value is obtained by putting

$$n_x = n_y = n_z = 1$$

$$\therefore \qquad E_{111} = \frac{3\,\pi^2\,\hbar^2}{2\,m\,a^2} \qquad \text{...(17)}$$

There is only one set of quantum numbers that gives this energy state, and this level is said to be *non-degenerate*.

There are three possibilities for the first excited state :

$$n_x = 2 \qquad n_y = n_z = 1$$

$$n_y = 2 \qquad n_x = n_z = 1$$

$$n_z = 2 \qquad n_x = n_y = 1$$

$$E_{211} = E_{121} = E_{112} = \frac{3\,\pi^2\,\hbar^2}{ma^2} \qquad \text{...(18)}$$

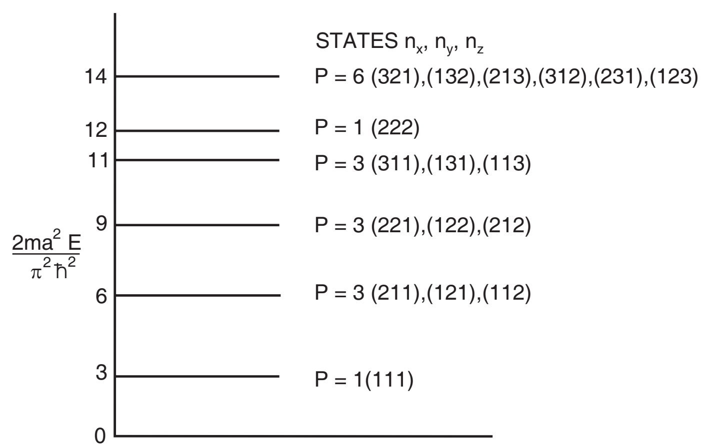


Fig. 5.10

Here there are three sets (211), (121) and (112) of the quantum numbers n_x, n_y, and n_z that will give the same energy level. That is, several distinct quantum states possess the same energy. This property is called *degeneracy*. In this particular case, the level is *triply degenerate*. Fig. 5.10 shows energy levels, degree of degeneracy and quantum numbers of a particle in a cubical box.

Eq. (15) indicates that the energy values of a particle in an infinitely deep potential well are not continuous but *discrete*. The particle has different bound states inside the well.

5.6 LINEAR HARMONIC OSCILLATOR

Consider a particle executing simple harmonic motion along the x direction (Fig. 5.11).

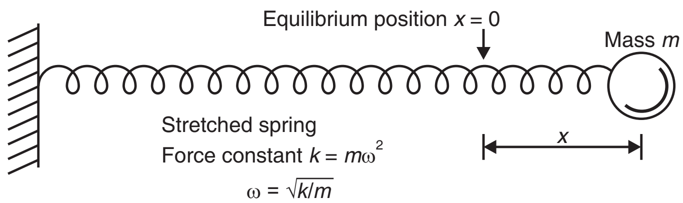


Fig. 5.11

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 Schrödinger equation for the harmonic oscillator is

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

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

$$y = \left(\frac{1}{\hbar}\sqrt{km}\right)^{1/2} x = \sqrt{\frac{2\pi m\nu}{\hbar}}\, x \qquad ...(2)$$

and

$$\alpha = \frac{2E}{\hbar}\sqrt{\frac{m}{k}} = \frac{2E}{h\nu} \qquad ...(3)$$

where ν is the classical frequency of the oscillation given by

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

In terms of y and α, Schrödinger'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:

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

Here, $f(y)$ is a function of y that remains to be found.

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

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

which is the differential equation that *f* obeys.

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

$$\frac{d^2 f}{dy^2} - 2y\frac{df}{dy} + 2nf = 0. \quad ...(7)$$

This is a standard mathematical equation known as *Hermite's equation.*

The solutions of Eq. (7) are called *Hermite's Polynomials*, given by

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

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

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

Here, N is a normalisation constant.

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

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

The energy of a harmonic oscillator is thus quantised in steps of $h\nu$. The energy levels here are evenly spaced (Fig. 5.12).

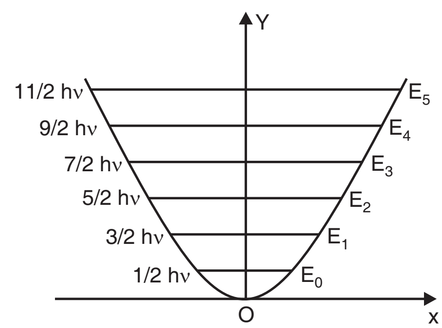


Fig. 5.12

Zero-point energy. When $n = 0$, $E_o = \frac{1}{2}h\nu$.

This is the lowest value of energy the oscillator can have. This value is called the *zero point energy*.

Wave Functions. Each wave function ψ_n consists of a polynomial $H_n(y)$ (called a *Hermite polynomial*), the exponential factor $e^{-y^2/2}$ and a numerical coefficient which is needed for ψ_n to meet the normalisation condition

$$\int_{-\infty}^{\infty} |\psi_n|^2 \, dy = 1 \quad n = 0, 1, 2, ... \quad ...(11)$$

The general formula for the nth wave function is

$$\psi_n = \left(\frac{2m\nu}{h/2\pi}\right)^{1/4} (2^n n!)^{-1/2} H_n(y) e^{-y^2/2} \quad ...(12)$$

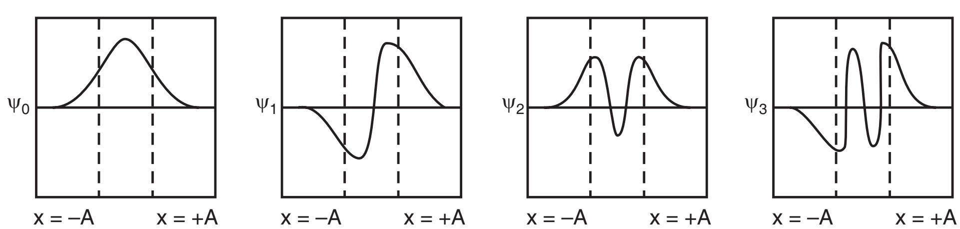


Fig. 5.13

The first four Hermite polynomials H_n (y) are listed in Table 8.1. The corresponding wave functions are plotted in Fig. 5.13. The vertical lines show the limits $-A$ and $+A$ between which a classical oscillator with the same energy would vibrate.

n	H_n (y)	E_n
0	1	$\frac{1}{2}h\nu$
1	$2y$	$\frac{3}{2}h\nu$
2	$4y^2 - 2$	$\frac{5}{2}h\nu$
3	$8y^3 - 12y$	$\frac{7}{2}h\nu$

5.7 THREE DIMENSIONAL HARMONIC OSCILLATOR—(SPHERICALLY SYMMETRIC CASE)

A three dimensional harmonic oscillator consists of a particle bound to origin by a force proportional to the displacement r from the fixed point, *i.e.*,

$$F = -kr.$$

Here, k is force constant.

We consider the special case in which frequency of oscillator along three axes X, Y and Z are same, *i.e.*,

$$\nu_x = \nu_y = \nu_z = \nu \text{ (say)}$$

$$\therefore \quad k = m\omega^2 = m\,(2\pi\nu)^2 = 4\pi^2\,\nu^2\,m. \quad \text{...(1)}$$

Potential energy of oscillator assuming zero potential energy at $r = 0$ is

$$V = -\int F\,dr = \int kr\,dr = \frac{1}{2}kr^2$$

But

$$r^2 = x^2 + y^2 + z^2$$

$$\therefore \quad V(r) = \frac{1}{2}kr^2 = \frac{1}{2}k\,(x^2 + y^2 + z^2).$$

The Schrödinger equation for this system is

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial\ \psi}{\partial z^2} \quad \frac{2m}{\hbar^2}\left[E - \frac{1}{2}k\,(x^2 + y^2 + z^2)\right]\psi = 0$$

or

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial\ \psi}{\partial z^2} \quad 2\sqrt{\frac{m}{\hbar^2}}\sqrt{\frac{mk}{\hbar^2}}$$

$$\times\left[\frac{E}{\sqrt{k}} - \frac{1}{2}\sqrt{k}\,(x^2 + y^2 + z^2)\right]\psi = 0.$$

or

$$\frac{1}{\sqrt{\frac{mk}{\hbar^2}}}\left\{\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial\ \psi}{\partial z^2}\right\}$$

$$+\left\{2\sqrt{\frac{m}{\hbar^2\,k}}\,E - \sqrt{\frac{mk}{\hbar^2}}\,(x^2 + y^2 + z^2)\right\}\psi = 0 \quad \text{...(2)}$$

5.8 POTENTIAL STEP

The potential function of a potential step is defined by

$$V(x) = 0 \qquad x < 0$$
$$= V_0 \qquad x > 0 \qquad ...(1)$$

Let electrons of energy E move from left to right, *i.e.*, along the positive direction of x-axis (Fig. 5.14). It is desired to find the eigenfunction solutions of the time-independent Schrödinger equation

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

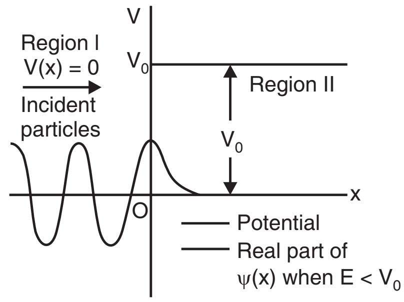


Fig. 5.14

For I region $V(x) = 0$. Therefore, the Schrödinger equation takes the form

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad ...(3)$$

The solution of Eq. (3) is

$$\psi_1 = Ae^{ip_1 x/\hbar} + Be^{-ip_1 x/\hbar} \qquad ...(4)$$

where A and B are constants.

$$p_1 = \sqrt{(2mE)}.$$

Some particles may be reflected by the potential barrier and some transmitted. The first and second terms respectively represent the *incident* and *reflected* particles.

The Schrödinger wave equation for II region is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\,\psi = 0 \qquad ...(5)$$

The solution of Eq. (5) is

$$\psi_2 = Ce^{ip_2 x/\hbar} + De^{-ip_2 x/\hbar} \qquad ...(6)$$

where $p_2 = \sqrt{[2m(E - V_0)]}$; C and D are constants.

In Eq. (6), the first term represents the *transmitted wave.* The second term represents a wave coming from $+\infty$ in the negative direction. Clearly for $x > 0$ no particles can flow to the left and D must be zero. Therefore, Eq. (6) becomes

$$\psi_2 = Ce^{ip_2 x/\hbar} \qquad ...(7)$$

The continuity of ψ implies that $\psi_1 = \psi_2$ at $x = 0$

$$\therefore \qquad A + B = C. \qquad ...(8)$$

The continuity of $\frac{d\psi}{dx}$ implies that $\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$ at $x = 0$.

$$\therefore \qquad p_1(A - B) = p_2 C \qquad ...(9)$$

Solving (8) and (9) we get

$$B = \frac{p_1 - p_2}{p_1 + p_2}A \qquad ...(10)$$

and

$$C = \frac{2p_1}{p_1 + p_2}A \qquad ...(11)$$

B and C represents the amplitudes of *reflected* and *transmitted* beams respectively in terms of the amplitude of the incident wave.

The *reflectance* and the *transmittance* at the potential discontinuity may be defined as follows:

$$\text{Reflectance} \quad R = \frac{\text{magnitude of reflected current}}{\text{magnitude of incident current}}$$

$$\text{Transmittance} \quad T = \frac{\text{magnitude of transmitted current}}{\text{magnitude of incident current}}$$

Two cases may arise : (*i*) $E > V_0$ and (*ii*) $E < V_0$

Case (i): $E > V_0$. When $E > V_0$, $p_2 = \sqrt{[2m(E-V_0)]}$ is real.

We will now derive expressions for the current density in the I and II regions.

The *probability current* is defined as

$$J = \frac{\hbar}{2im}[\psi^* \nabla \psi - \psi \nabla \psi^*] \qquad ...(12)$$

$$\therefore \quad (J_x)_1 = \frac{\hbar}{2im}\left[\psi^*_1 \frac{d\psi_1}{dx} - \psi_1 \frac{d\psi_1^*}{dx}\right]$$

$$= \frac{\hbar}{2im}\left[\left\{\left(A^* e^{-ip_1x/\hbar} + B^* e^{ip_1x/\hbar}\right) \times \left(\frac{ip_1}{\hbar}\right)\left(Ae^{ip_1x/\hbar} - Be^{-ip_1x/\hbar}\right)\right\} - \left\{\left(Ae^{ip_1x/\hbar} + Be^{-ip_1x/\hbar}\right) \times \left(-\frac{ip_1}{\hbar}\right)\left(A^* e^{-ip_1x/\hbar} - B^* e^{ip_1x/\hbar}\right)\right\}\right]$$

$$= \frac{p_1\,(AA^* - B^*B)}{m} = \frac{p_1}{m}\left[|A|^2 - |B|^2\right] \qquad ...(13)$$

From the above relation it is evident that the current in the I region is equal to the difference between two terms. The first term which is proportional to $p_1\,|A|^2$ represents the *incident wave.* The second term which is proportional to $p_1|B|^2$ represents the *reflected wave.*

$$\left.\begin{array}{l}\text{The probability current}\\ \text{of the incident beam}\end{array}\right\} = |A|^2\,\frac{p_1}{m} \qquad ...(14)$$

$$\left.\begin{array}{l}\text{The probability current}\\ \text{of the reflected beam}\end{array}\right\} = |B|^2\,\frac{p_1}{m} \qquad ...(15)$$

The expression for the probability current in region II is

$$(J_x)_{\text{II}} = \frac{\hbar}{2im}\left[\psi_2{}^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx}\right]$$

$$= \frac{\hbar}{2im}\left[\left\{C^* e^{-ip_2x/\hbar}\left(\frac{ip_2}{\hbar}\right)Ce^{ip_2x/\hbar}\right\} - \left\{Ce^{ip_2x/\hbar}\left(-\frac{ip_2}{\hbar}\right)C^* e^{-ip_2x/\hbar}\right\}\right]$$

$$= \frac{p_2}{2m}\left[CC^* + CC^*\right] = \frac{p_2}{m}(CC^*)$$

$$= \frac{|C|^2\, p_2}{m} \qquad \text{...(16)}$$

Eq. (16) represents the *transmitted current.*

$$R = \frac{\text{magnitude of reflected current}}{\text{magnitude of incident current}}$$

$$= \frac{|B|^2\,(p_1/m)}{|A|^2\,(p_1/m)}$$

$$R = \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2} \text{ from Eq. (10)} \qquad \text{...(17)}$$

$$T = \frac{\text{magnitude of transmitted current}}{\text{magnitude of incident current}}$$

$$= \frac{|C|^2\,(p_2/m)}{|A|^2\,(p_1/m)}$$

$$= \left(\frac{2\,p_1}{p_1 + p_2}\right)^2 \times \frac{p_2}{p_1} \text{ from Eq. (11)}$$

$$\therefore \quad T = \frac{4 p_1 p_2}{(p_1 + p_2)^2} \qquad \text{...(18)}$$

Case (ii). $E < V_0$. When $E < V_0$, $p_2 = \sqrt{[2m(E - V_0)]}$ is imaginary.

Hence $p_2 = i\sqrt{[2m(V_0 - E)]}$ and $p_2^* = -i\sqrt{[2m(V_0 - E)]} = -p_2$.

The probability current in this case is given by

$$J_x = \frac{\hbar}{2im}\left[\psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx}\right]$$

$$= \frac{\hbar}{2im}\left[C^* e^{-ip_2^* x/\hbar}\left(\frac{ip_2}{\hbar}\right) C\, e^{ip_2 x/\hbar} - C e^{ip_2 x/\hbar}\left(-\frac{ip_2^*}{\hbar}\right) C^* e^{-ip_2^* x/\hbar}\right]$$

Substituting $p_2^* = -p_2$ we get,

$$J_x = \frac{\hbar}{2im}\left[C^* e^{ip_2 x/\hbar}\left(\frac{ip_2}{\hbar}\right) C\, e^{ip_2 x/\hbar} - CC^*\left(\frac{ip_2}{\hbar}\right) e^{ip_2 x/\hbar} e^{ip_2 x/\hbar}\right]$$

$$= 0$$

Thus the transmitted current is zero.

$$T = \frac{\text{magnitude of transmitted current}}{\text{magnitude of incident current}} = 0$$

$$\therefore \quad T = 0 \qquad \text{...(19)}$$

By definition, $R + T = 1$

$$\therefore \quad R = 1 \qquad \text{...(20)}$$

5.9 THE BARRIER PENETRATION PROBLEM

Consider a beam of particles of kinetic energy E incident from the left on a potential barrier of height V and width $OA = L$ (Fig. 5.15). $V > E$ and on both sides of the barrier, $V = 0$, which means that no forces act upon the particles there. This potential is described by

$V = 0$ for $x < 0$ (region I)

$V = V$ for $0 < x < L$ (region II)

$V = 0$ for $x > L$ (region III) ...(1)

Let ψ_1, ψ_2, and ψ_3 be the respective wave functions in regions I, II and III as indicated in the figure.

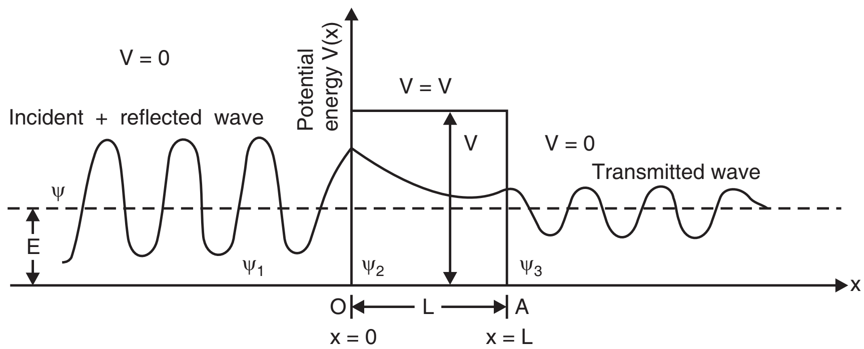


Fig. 5.15

The corresponding Schrödinger equations are

region I $\quad \dfrac{d^2\psi_1}{dx^2}+\dfrac{2mE}{\hbar^2}\psi_1 = 0 \quad$ since $V = 0$

region II $\quad \dfrac{d^2\psi_2}{dx^2}+\dfrac{2m}{\hbar^2}(E-V)\psi_2 = 0 \quad (\because\ V = V)$

region III $\quad \dfrac{d^2\psi_3}{dx^2}+\dfrac{2mE}{\hbar^2}\psi_3 = 0 \quad (\because\ V = 0)$ ...(2)

Put $\dfrac{2mE}{\hbar^2} = \alpha^2$ and $\dfrac{2m}{\hbar^2}(V-E)= \beta^2$.

Then the equations become

region I $\quad \dfrac{d^2\psi_1}{dx^2}+\alpha^2\psi_1 = 0$

region II $\quad \dfrac{d^2\psi_2}{dx^2}-\beta^2\psi_2 = 0$ ...(3)

region III $\quad \dfrac{d^2\psi_3}{dx^2}+\alpha^2\psi_3 = 0$

The solutions to these equations are

region I $\quad \psi_1 = Ae^{i\alpha x}+Be^{-i\alpha x}$

region II $\quad \psi_2 = Fe^{-\beta x}+Ge^{\beta x}$ ...(4)

region III $\psi_3 = Ce^{i\alpha x} + De^{-i\alpha x}$

where the constants *A, B* and so on are the amplitudes of the corresponding components of each wave. They may be recognized as follows:

A is the amplitude of the wave, incident on the barrier from the left,

B is the amplitude of the reflected wave in region I,

F is the amplitude of the wave, penetrating the barrier in region II,

G is the amplitude of the reflected wave (from the surface at *A*) in region II,

C is the amplitude of the transmitted wave, in region III, and

D is the amplitude of a (nonexistent) reflected wave, in region III.

It should be noted that we have drawn the wave function through the three regions in Fig. 8.12 so that it is continuous and singly valued everywhere along the *x*-axis.

Since the probability density associated with a wave function is proportional to the square of the amplitude of that function, we can define the barrier transmission coefficient as

$$T = \frac{|C|^2}{|A|^2} \qquad \text{...(5)}$$

and a reflection coefficient for the barrier surface at $x = 0$ as

$$R = \frac{|B|^2}{|A|^2} \qquad \text{...(6)}$$

If the barrier is high, compared to the total energy of the particle, or is thick compared to the wavelength of the wave function, then the transmission coefficient becomes

$$T \approx 16\frac{E}{V}\left(1-\frac{E}{V}\right)\exp\left[-\frac{2L}{\hbar}\sqrt{2m\,(V-E)}\right] \qquad \text{...(7)}$$

where *L* is the physical thickness of the barrier. The ratio $\frac{|C|^2}{|A|^2}$ is also called the 'penetrability' of the barrier. It represents the probability that a particle incident on the barrier from one side will appear on the other side. Such a probability is zero classically, but a finite quantity in quantum mechanics. We thus conclude that if a particle with energy *E* is incident on a thin energy barrier of height greater than *E*, there is a finite probability of the particle penetrating the barrier. This phenomenon is called the *tunnel effect*. This effect was used by George Gamow in 1928 to explain the process of α-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.

Sol. From equation (7), the transmission coefficient is

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

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

$$\approx 0.084$$

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

Calculation of Transmission Coefficient T

The arbitrary constants A, B, F, G and C are found from the boundary conditions at $x = 0$ and $x = L$.

The wave function and its derivative must be continuous at $x = 0$ and $x = L$.

$$\psi_1 = A e^{i\alpha x} + B e^{-i\alpha x}$$
$$\psi_2 = F e^{-\beta x} + G e^{\beta x}$$
$$\psi_3 = C e^{i\alpha x}$$

At $x = 0$, $\psi_1(0) = \psi_2(0)$. $\therefore$ $A + B = F + G$ ...(1)

At $x = 0$, $\psi_1'(0) = \psi_2'(0)$. $\therefore$ $i\alpha(A - B) = -\beta(F - G)$

or $$A - B = \frac{i\beta}{\alpha}(F - G) \quad ...(2)$$

At $x = L$, $\psi_2(L) = \psi_3(L)$ $\therefore$ $F e^{-\beta L} + G e^{\beta L} = C e^{i\alpha L}$ ...(3)

At $x = L$, $\psi_2'(L) = \psi_3'(L)$

$$\therefore \quad -\beta[F e^{-\beta L} - G e^{\beta L}] = i\alpha C e^{i\alpha L} \quad ...(4)$$

Solving for F and G we get

$$F = \frac{C}{2} e^{i\alpha L}\left(1 - \frac{i\alpha}{\beta}\right) e^{\beta L} = \frac{C}{2\beta}(\beta - i\alpha)\, e^{i\alpha L}\, e^{\beta L}$$

$$G = \frac{C}{2} e^{i\alpha L}\left(1 + \frac{i\alpha}{\beta}\right) e^{-\beta L} = \frac{C}{2\beta}(\beta + i\alpha)\, e^{i\alpha L}\, e^{-\beta L}$$

Using Eqs. (1) and (2) we get

$$A = \frac{C}{4} e^{i\alpha L}\left[-\frac{(\beta - i\alpha)^2}{i\alpha\beta} e^{\beta L} + \frac{(\beta + i\alpha)^2}{i\alpha\beta} e^{-\beta L}\right]$$

$$\frac{C}{A} = \frac{4i\alpha\beta e^{-i\alpha L}}{(\beta + i\alpha)^2 e^{-\beta L} - (\beta - i\alpha)^2 e^{\beta L}}$$

$$= \frac{4i\alpha\beta e^{-i\alpha L}}{2(\alpha^2 - \beta^2)\sinh\beta L + 4i\alpha\beta\cosh\beta L}$$

$$\therefore \quad \left|\frac{C}{A}\right|^2 = \frac{4\alpha^2\beta^2}{(\alpha^2 - \beta^2)^2\sinh^2\beta L + 4\alpha^2\beta^2\cosh^2\beta L}$$

$$= \frac{4\alpha^2\beta^2}{4\alpha^2\beta^2 + (\alpha^2 + \beta^2)^2\sinh^2\beta L}$$

$$\therefore \quad T = \left|\frac{C}{A}\right|^2 = \left[1 + \frac{(\alpha^2 + \beta^2)^2}{4\alpha^2\beta^2}\sinh^2\beta L\right]^{-1}$$

But $$(\alpha^2 + \beta^2)^2 = \left(\frac{2m}{\hbar^2}\right)^2 V^2, \quad \alpha^2\beta^2 = \left(\frac{2m}{\hbar^2}\right)^2 E(V - E)$$

$$\therefore \qquad T = \left[1 + \frac{V^2}{4E(V-E)}\sinh^2 \beta L\right]$$

If βL is large, then $\sinh \beta L$ behaves as $e^{\beta L}/2$.

$$\sinh^2 \beta L \approx \frac{1}{4}e^{2\beta L} >> 1; \quad \beta = \frac{\sqrt{2m(V-E)}}{\hbar}$$

$$\therefore \qquad T = 16\frac{E}{V}\left(1-\frac{E}{V}\right)e^{-\frac{2L}{\hbar}\sqrt{2m(V-E)}}$$

5.10 Tunnel Effect

Consider a potential barrier of height V, with $E < V$.

The barrier has a finite width (Fig. 5.16).

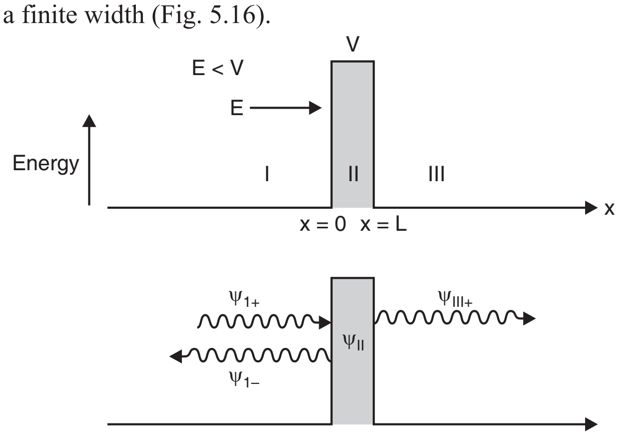


Fig. 5.16

The de Broglie waves that correspond to the particle are partly refected and partly transmitted.

This means that the particle has a finite chance of penetrating the barrier.

The particle has a certain probability of passing through the barrier and emerging on the other side. The particle lacks the energy to go over the top of the barrier. But the particle can tunnel through the walls. The higher the barrier and the wider it is, the less the chance that the particle can get through.

Explanation of Alpha Decay

The decay of a nucleus by alpha particle emission is explained on the basis of quantum tunneling. An α-particle whose kinetic energy is only a few MeV is able to escape from nucleus whose potential wall is 25 MeV high. The probability of escape is so small that the α-particle might have to strike the wall 10^{38} or more times before it emerges. But sooner or later it does get out.

Approximate transmission probability

Consider a beam of identical particles all of which have the kinetic energy E. The beam is incident from region I on a potential barrier of height V and width L (Fig. 8.13). On both sides of the barrier $V = 0$.

This means that no forces act on particles in regions I and III.

- The wave function ψ_{I+} represents the incoming particles moving towards the barrier from region I.
- The wave function ψ_{I-} represents the reflected particles moving to the left away from the barrier.

- The wave function ψ_{III} represents the transmitted particles moving to the region III.

The transmission probability T for a particle to pass through the barrier is given by

$$T = \frac{\text{Number of particles transmitted}}{\text{Number of particles incident}}.$$

This probability is approximately given by

$$T = \exp\left[-\frac{2L}{\hbar}\sqrt{2m(V-E)}\right]$$

EXERCISE

1. Arrive at the time-dependent Schrödinger's equation.
2. Derive one dimensional time independent Schrödinger wave equation.
3. What do you understand by Eigen value and Eigen function?
4. Explain the physical interpretation of wave function.
5. What is wave function? Discuss the properties of wave functions.
6. Explain the normalization and orthogonality of wave function.
7. Calculate the values of energy of a particle in a one-dimensional box. Graphically indicate some of the wave functions for such a particle.
8. Discuss quantum mechanically the problem of a particle in a finite square potential well. Draw diagrams showing the amplitude wave and probability density for the same. What will be the effect of increasing the width of the square well on energy levels?
9. Obtain the time independent Schrödinger's equation and solve it in the case of a particle in one dimensional rectangular potential well of finite depth.
10. (*a*) Write Schrödinger's equation for a particle in a rigid box and solve it. Find the eigen functions when a particle is kept in a rectangular box of dimensions $l_x \times l_y \times l_z$. Find the eigen values of momentum and energy.

    (*b*) Show that for a single value of energy or momentum, different quantum states are possible. Explain the term degeneracy.
11. What is potential step? Find the reflection and transmission co-efficient for potential step of the form $0 < E < V_0$. Show that there is a finite probability of locating the particle in the region which is forbidden classically. What is the penetration distance? Give its relation to the mass of the incident particle.
12. What is tunnel effect? Give any two examples.
13. A particle of mass m and energy $E < V_0$ travelling along x-axis has a potential barrier defined by

$$V(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ V_0 & \text{for} \quad 0 < x < a \\ 0 & \text{for} \quad x > a \end{cases}$$

Derive the expression for reflection and transmission co-efficient of the particle.

14. Formulate the Schrödinger's equation for a linear harmonic oscillator and solve it to obtain its eigen values and eigen function.
15. Find the solution of three dimensional harmonic oscillator in rectangular coordinates.
16. Discuss the rigid rotator problem in wave mechanics and arrive at the eigen value of it.