

Classical Mechanics

1 Mechanics Of a Particle

1.1 Conservation theorem for linear momentum of a particle.

Statement:- If the sum of external forces acting on a particle is zero, then the linear momentum of the particle is conserved.

Proof:- Consider a particle acted upon by a force \vec{F} . Then according to Newton's second law of motion, we have

$$\frac{d\vec{P}}{dt} = \vec{F} \quad \text{where } \vec{P} \text{ is the linear momentum of the particle.}$$

Thus if the external force $\vec{F} = 0$ then $\frac{d\vec{P}}{dt} = 0$ or $\vec{P} = \text{constant of time}$. In other word, if the sum of external forces acting on the particle is zero, then the linear momentum of the particle is conserved.

1.2 Conservation theorem for angular momentum of a particle.

Statement:- If the total moment of the forces or torque acting on a particle is zero, then the angular momentum of the particle is conserved.

Proof:- If \vec{P} is the linear momentum of the particle and \vec{r} is the radius vector from the arbitrary origin 'O' then the angular momentum of the particle about the origin is

$$\vec{L} = \vec{r} \times \vec{P} = \vec{r} \times m\vec{v}$$

where m is the mass and \vec{v} is the velocity of the particle.

Differentiating the above equation with respect to time, we get

$$\frac{d\vec{L}}{dt} = \frac{d}{dt} [\vec{r} \times m\vec{v}] = \left[\frac{d\vec{r}}{dt} \times m\vec{v} \right] + \left[\vec{r} \times \frac{d(m\vec{v})}{dt} \right] = [\vec{v} \times m\vec{v}] + \left[\vec{r} \times \frac{d(m\vec{v})}{dt} \right]$$

$$\text{or } \frac{d\vec{L}}{dt} = 0 + \left[\vec{r} \times \frac{d(m\vec{v})}{dt} \right] = \vec{r} \times \frac{d\vec{P}}{dt} = \vec{r} \times \vec{F}$$

where \vec{F} is the total force acting on the particle.

$$\text{or } \frac{d\vec{L}}{dt} = \vec{N}$$

where $\vec{N} = \vec{r} \times \vec{F}$ is the moment of the force or torque acting on the particle.

Thus, if $\vec{N} = 0$ then $\frac{d\vec{L}}{dt} = 0$ or $\vec{L} = \text{constant of time}$.

It implies that, if the moment of the total force or torque acting on a particle is zero, then the angular momentum of the system is conserved. Hence the proof.

1.3 Conservation theorem for total energy of a particle.

Statement:- If the forces acting on a particle are conservative then the total energy of the particle is conserved.

Proof:- Suppose a particle is acted under action of a conservative force \vec{F} and is moved from position 1 to position 2. Then the work done under this process is

$$W_{12} = \int_1^2 \vec{F} \cdot d\vec{r} = \int_1^2 \frac{d\vec{P}}{dt} \cdot d\vec{r} = \int_1^2 \frac{d(m\vec{v})}{dt} \cdot d\vec{r} \quad (1)$$

Now consider the term

$$\vec{v} = \frac{d\vec{r}}{dt} \quad \text{or } d\vec{r} = \vec{v} dt$$

Using it in the above equation, we get

$$W_{12} = \int_1^2 \frac{d(m\vec{v})}{dt} \cdot d\vec{r} = \int_1^2 \frac{d(m\vec{v})}{dt} \cdot \vec{v} dt \quad (2)$$

Further $\frac{dv^2}{dt} = \frac{d}{dt}(\vec{v} \cdot \vec{v}) = \frac{d\vec{v}}{dt} \cdot \vec{v} + \vec{v} \cdot \frac{d\vec{v}}{dt} = 2 \frac{d\vec{v}}{dt} \cdot \vec{v}$

or $\frac{d\vec{v}}{dt} \cdot \vec{v} = \frac{1}{2} \frac{dv^2}{dt}$

or $\frac{d(m\vec{v})}{dt} \cdot \vec{v} = \frac{d\left(\frac{1}{2}mv^2\right)}{dt}$

Substituting it in equation (2), we get

$$W_{12} = \int_1^2 \frac{d\left(\frac{1}{2}mv^2\right)}{dt} dt = \int_1^2 d\left(\frac{1}{2}mv^2\right) = \int_1^2 dT = T_2 - T_1 \quad (3)$$

where T_1 and T_2 represent the initial and final kinetic energies of the particle respectively.

If the force \vec{F} acting on the particle is conservative then

$$\vec{F} = -\nabla V$$

where V is the potential energy of the particle.

The work done in displacing the system from position 1 to position 2 under action of this force is given by

$$W_{12} = \int_1^2 \vec{F} \cdot d\vec{r} = -\int_1^2 \nabla V \cdot d\vec{r} = -\int_1^2 \frac{\partial V}{\partial r} dr = -\int_1^2 dV = -V_2 + V_1 \quad (4)$$

where V_1 and V_2 represent the initial and final potential energies of the particle respectively.

Equating equations (3) and (4), we get

$$T_2 - T_1 = -V_2 + V_1$$

or $T_2 + V_2 = T_1 + V_1$

or $T + V = \text{constant}$

Thus, if the forces acting on a particle are conservative then the total energy of the particle is conserved. Hence the proof.

2 MECHANICS OF A SYSTEM OF PARTICLES

2.1 Centre of mass of a system of particles:

If a system consists of n number of particles of masses m_1, m_2, \dots, m_n whose position vectors from any arbitrary origin 'O' are $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n$ respectively, then the centre of mass of the system defined as the geometrical point whose position vector is given by

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2 + \dots + m_n\vec{r}_n}{m_1 + m_2 + \dots + m_n} = \frac{\sum_i m_i \vec{r}_i}{\sum_i m_i}$$

or $\vec{R} = \frac{\sum_i m_i \vec{r}_i}{M}$

where $M = \sum_i m_i$ is the total mass of the system.

2.2 Conservation theorem for linear momentum of a system of particles.

Statement:- If the sum of external forces acting on a system of particles is zero, then the total linear momentum of the system is conserved.

Proof:- Consider a system of finite number of particles acted upon by various forces. Any given particle of the system will experience two types of forces: 1) the external force due to the agent outside the system

and 2) internal forces due to the other particles of the system. Thus the total force \vec{F}_i acting on the i^{th} particle can be written as

$$\vec{F}_i = \vec{F}_i^e + \sum_j \vec{F}_{ji} \quad (1)$$

where \vec{F}_i^e stands for an external force and \vec{F}_{ji} is the internal force on the i^{th} particle due to the j^{th} particle.

Obviously, $\vec{F}_{ii} = 0$.

The equation for motion for the i^{th} particle can be written as

$$\frac{d\vec{P}_i}{dt} = \vec{F}_i$$

$$\text{or} \quad \frac{d\vec{P}_i}{dt} = \vec{F}_i^e + \sum_j \vec{F}_{ji}$$

Summing over all the particles, we get

$$\begin{aligned} \sum_i \frac{d\vec{P}_i}{dt} &= \sum_i \vec{F}_i^e + \sum_i \sum_j \vec{F}_{ji} \\ \frac{d}{dt} \sum_i \vec{P}_i &= \sum_i \vec{F}_i^e + \sum_{i,j} \vec{F}_{ji} \end{aligned} \quad (2)$$

Now $\sum_i \vec{F}_i^e = \vec{F}^e$ is simply the total external force and $\sum_{i,j} \vec{F}_{ji} = 0$ since the law of action and reaction

states that each pair $\vec{F}_{ji} + \vec{F}_{ij}$ equal to zero.

Thus equation (2) becomes

$$\frac{d}{dt} \sum_i \vec{P}_i = \vec{F}^e \quad \text{or} \quad \frac{d\vec{P}}{dt} = \vec{F}^e$$

where $\sum_i \vec{P}_i = \vec{P}$ is the total linear momentum of the system.

If $\vec{F}^e = 0$ then $\frac{d\vec{P}}{dt} = 0$ or $\vec{P} = \text{constant}$ with time.

Thus, if the sum of external forces acting on a system of particles is zero, then the total linear momentum of the system is conserved. Hence the proof.

2.3 Conservation theorem for angular momentum of a system of particles.

Statement:- If the total moment of the external forces acting on a system of particles is zero, then the total angular momentum of the system is conserved.

Proof:- Consider a system of finite number of particles. The angular momentum of i^{th} particle of the system about any origin 'O' is given by

$$\vec{L}_i = \vec{r}_i \times \vec{P}_i \quad (1)$$

where \vec{r}_i is the radius vector and \vec{P}_i is the linear momentum of the particle. Further, $\vec{P}_i = m_i \vec{v}_i$ with \vec{v}_i is the velocity and m_i is the mass of the i^{th} particle. Using this equation (1) becomes

$$\vec{L}_i = \vec{r}_i \times m_i \vec{v}_i$$

Differentiating it with respect to time, we get

$$\begin{aligned} \frac{d}{dt} \vec{L}_i &= \frac{d}{dt} [\vec{r}_i \times m_i \vec{v}_i] = \left[\frac{d\vec{r}_i}{dt} \times m_i \vec{v}_i \right] \\ &+ \left[\vec{r}_i \times \frac{d(m_i \vec{v}_i)}{dt} \right] = [\vec{v}_i \times m_i \vec{v}_i] + \left[\vec{r}_i \times \frac{d(m_i \vec{v}_i)}{dt} \right] \end{aligned}$$

$$\text{or } \frac{d\vec{L}_i}{dt} = 0 + \left[\vec{r}_i \times \frac{d(m_i \vec{v}_i)}{dt} \right]$$

$$\text{or } \frac{d\vec{L}_i}{dt} = \vec{r}_i \times \frac{d(m_i \vec{v}_i)}{dt} = \vec{r}_i \times \frac{d\vec{P}_i}{dt}$$

$$\text{or } \frac{d\vec{L}_i}{dt} = \vec{r}_i \times \vec{F}_i$$

where $\vec{F}_i = \frac{d\vec{P}_i}{dt}$ is the total force acting on the i^{th} particle.

$$\text{or } \frac{d\vec{L}_i}{dt} = \vec{N}_i$$

where $\vec{N}_i = \vec{r}_i \times \vec{F}_i$ is the moment of total force or total torque acting on the i^{th} particle.

Summing over all particles of the system, we get

$$\sum_i \frac{d\vec{L}_i}{dt} = \sum_i \vec{N}_i$$

$$\text{or } \frac{d}{dt} \sum_i \vec{L}_i = \sum_i \vec{N}_i \quad \text{or} \quad \frac{d}{dt} \vec{L} = \sum_i \vec{N}_i \quad (2)$$

where $\vec{L} = \sum_i \vec{L}_i$ is the total angular momentum of the system.

Now consider,

$$\sum_i \vec{N}_i = \sum_i \vec{r}_i \times \vec{F}_i = \sum_i \vec{r}_i \times \left(\vec{F}_i^e + \sum_j \vec{F}_{ji} \right)$$

where \vec{F}_i^e stands for an external force on i^{th} particle and \vec{F}_{ji} is the internal force on i^{th} particle due to j^{th} particle. Thus,

$$\sum_i \vec{N}_i = \sum_i \vec{r}_i \times \vec{F}_i^e + \sum_{i,j} \vec{r}_i \times \vec{F}_{ji} \quad (3)$$

The second term on RHS of this equation vanishes according to the law of action and reaction as the internal forces occur in equal and opposite pairs. Therefore, we have

$$\sum_i \vec{N}_i = \sum_i \vec{r}_i \times \vec{F}_i^e = \sum_i \vec{N}_i^e = \vec{N}^e$$

where $\sum_i \vec{N}_i^e = \vec{N}^e$ is the total moment of the external force or total external torque on the system.

Substituting it in equation (2), we get

$$\frac{d\vec{L}}{dt} = \vec{N}^e$$

Thus, if $\vec{N}^e = 0$ then $\frac{d\vec{L}}{dt} = 0$ or $\vec{L} = \text{constant with time.}$

It implies that, if the total moment of the external forces acting on a system of particles is zero, then the total angular momentum of the system is conserved. Hence the proof.

2.4 Conservation theorem for total energy of a system of particles.

Statement:- If the forces acting on a system of particles are conservative then the total energy of the system is conserved.

Proof:- Consider a system of finite number of particles acted upon by conservative forces. Let W_{i12} be the work done in displacing i^{th} particle from position 1 to position 2 then

$$W_{i_{12}} = \int_1^2 \vec{F}_i \cdot d\vec{r}_i \quad (1)$$

where \vec{F}_i is the total force acting on i^{th} particle given by

$$\vec{F}_i = \vec{F}_i^e + \sum_j \vec{F}_{ji}$$

The force \vec{F}_i^e stands for an external force and \vec{F}_{ji} is the internal force on the i^{th} particle due to the j^{th} particle. Therefore,

$$W_{i_{12}} = \int_1^2 \left(\vec{F}_i^e + \sum_j \vec{F}_{ji} \right) \cdot d\vec{r}_i = \int_1^2 \vec{F}_i^e \cdot d\vec{r}_i + \int_1^2 \sum_j \vec{F}_{ji} \cdot d\vec{r}_i$$

Taking summation over all the particles, we get

$$W_{12} = \sum_i W_{i_{12}} = \sum_i \int_1^2 \vec{F}_i^e \cdot d\vec{r}_i + \sum_i \int_1^2 \sum_j \vec{F}_{ji} \cdot d\vec{r}_i$$

$$\text{or } W_{12} = \sum_i \int_1^2 \vec{F}_i^e \cdot d\vec{r}_i + \int_1^2 \sum_i \sum_j \vec{F}_{ji} \cdot d\vec{r}_i$$

$$\text{or } W_{12} = \sum_i \int_1^2 \vec{F}_i^e \cdot d\vec{r}_i + \int_1^2 \sum_{i,j} \vec{F}_{ji} \cdot d\vec{r}_i$$

As usual the last term on RHS vanishes because of the law of action and reaction. Therefore,

$$W_{12} = \sum_i \int_1^2 \vec{F}_i^e \cdot d\vec{r}_i = \sum_i \int_1^2 \frac{d\vec{p}_i}{dt} \cdot d\vec{r}_i = \sum_i \int_1^2 \frac{d\vec{p}_i}{dt} \cdot \vec{v}_i dt$$

$$\text{or } W_{12} = \sum_i \int_1^2 m_i \frac{d\vec{v}_i}{dt} \cdot \vec{v}_i dt \quad (2)$$

$$\text{But } \frac{d}{dt} (v_i^2) = \frac{d}{dt} (\vec{v}_i \cdot \vec{v}_i) = \frac{d\vec{v}_i}{dt} \cdot \vec{v}_i + \vec{v}_i \cdot \frac{d\vec{v}_i}{dt} = 2 \frac{d\vec{v}_i}{dt} \cdot \vec{v}_i$$

$$\text{or } \frac{d\vec{v}_i}{dt} \cdot \vec{v}_i = \frac{1}{2} \frac{d}{dt} (v_i^2) = \frac{d}{dt} \left(\frac{1}{2} v_i^2 \right)$$

Substituting it in equation (2), we get
or

$$\begin{aligned} W_{12} &= \sum_i \int_1^2 \frac{d}{dt} \left(\frac{1}{2} m_i v_i^2 \right) dt = \sum_i \int_1^2 d \left(\frac{1}{2} m_i v_i^2 \right) \\ &= \sum_i \int_1^2 dT_i = \sum_i [T_i]_1^2 \end{aligned}$$

$$\text{or } W_{12} = \sum_i [T_{i_2} - T_{i_1}] = \sum_i T_{i_2} - \sum_i T_{i_1}$$

$$\text{or } W_{12} = T_2 - T_1 \quad (3)$$

where T_1 and T_2 represent the initial and final kinetic energies of the system when it is displaced from position 1 to position 2 and W_{12} represents the net work done in this process.

If the external force \vec{F}_i^e acting on i^{th} particle is conservative then

$$\vec{F}_i^e = -\nabla V_i \quad (4)$$

where V_i is the potential energy of i^{th} particle.

The work done in displacing the system from position 1 to position 2 under action of this force is given by

$$W_{12} = \sum_i \int_1^2 \vec{F}_i^e \cdot d\vec{r}_i + \sum_{i,j} \int_1^2 \vec{F}_{ji} \cdot d\vec{r}_i$$

The last term vanishes as usual. Therefore,

$$W_{12} = \sum_i \int_1^2 \vec{F}_i^e \cdot d\vec{r}_i$$

Using equations (4), we get

$$W_{12} = -\sum_i \int_1^2 \nabla V_i \cdot d\vec{r}_i = -\sum_i \int_1^2 \frac{\partial V_i}{\partial r_i} dr_i = -\sum_i \int_1^2 dV_i = -\sum_i [V_i]_1^2$$

or
$$W_{12} = -\sum_i [V_{i2} - V_{i1}] = -\sum_i V_{i2} + \sum_i V_{i1}$$

or
$$W_{12} = -V_2 + V_1 \tag{5}$$

where V_1 and V_2 represent the initial and final potential energies of the system when it is displaced from position 1 to position 2.

Equating equations (3) and (5), we get

$$T_2 - T_1 = -V_2 + V_1$$

or
$$T_2 + V_2 = T_1 + V_1$$

or
$$T + V = \text{constant}$$

Thus, if the forces acting on a system of particles are conservative then the total energy of the system is conserved. Hence the proof.

3 Generalized Coordinates

The set of independent coordinates sufficient in numbers to specify the given systems configuration is called generalized coordinates and are denoted by $q_1, q_2, \dots, q_k, \dots, q_f$, where f is the total number of generalized coordinates called as the degree of freedom of the system.

Consider a system of n particles. There exists $3n$ number of independent coordinates. Suppose the motion of the system is restricted by holonomic constraints represented by l equations of the form

$$\begin{aligned} f_1(x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_n, y_n, z_n) &= 0 \\ f_2(x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_n, y_n, z_n) &= 0 \\ &\vdots \\ f_l(x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_n, y_n, z_n) &= 0 \end{aligned}$$

these l equations may be used to eliminate l of the $3n$ coordinates and now there are

$$(3n - l) = f \text{ (say) independent coordinates or degrees of freedom.}$$

Thus there exists

$$(3n - l) = f \text{ generalized coordinates.}$$

These generalized coordinates must satisfy the following conditions.

They must specify the configuration of the system.

They must be independent of each other.

They must simplify mathematical calculations without affecting informative solution.

4 Constraints:

Geometrical restrictions on the motion of a particle or a system of particles are known as constraints.

In practice the motion of a particle or a system of particles is generally restricted in some way. Some examples of these restrictions are:

The motion of rigid bodies is always such that the distance between any two particles remains unchanged.

The motion of a point mass of a simple pendulum is restricted since the point mass always remains at a constant distance from the point of suspension.

The motion of the gas molecules within a container is restricted by the wall of the vessel since gas molecules can move only inside the container.

4.1 Holonomic and Non-holonomic constraints:

Constraints may be classified into holonomic and non-holonomic as follows.

Let $\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_n$ be the position coordinates of a system and t denotes the time. If the conditions of all the constraints are expressed as equations of the form

$$f(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_n) = 0$$

then the constraints are said to be holonomic. If the conditions of the constraints are not so expressed then they are called non-holonomic constraints.

Examples of holonomic constraints:

The constraints involved in the motion of a rigid bodies in which the distance between any two particles is always fixed are holonomic, since the condition of constraints are expressed as

$$(\vec{r}_i - \vec{r}_j)^2 = c_{ij}^2 \quad \text{or} \quad (\vec{r}_i - \vec{r}_j) - c_{ij}^2 = 0$$

The constraints involved in the motion of the point mass of a simple pendulum are holonomic. In this case the point mass remains at a constant distance l from the point of suspension. If \vec{a} is the position vector of the point of suspension and \vec{r} is the position vector of the point mass then the condition of the constraint can be expressed as

$$(\vec{r} - \vec{a})^2 = l^2 \quad \text{or} \quad (\vec{r} - \vec{a})^2 - l^2 = 0$$

Examples of non-holonomic constraints:

The constraints involved in the motion a particle placed on the surface of a solid sphere are non-holonomic. The condition of constraints in this case may be expressed as

$$r^2 - a^2 \geq 0$$

Where a is the radius of the sphere and r is the distance of the particle from the centre of the sphere.

The constraints involved in the motion of the molecules of a gas contained in a container are non-holonomic.

The constraints are further classified into Scleronomic and Rheonomic. If the constraints are independent of time, they are termed as Scleronomic and if they are time-dependent then they are Rheonomic.

5 Principle of virtual work

Imagine two possible configurations of a system of particle at any time. If the system goes from one configuration to the other, each particle of the system is imagined to be displaced by an infinitesimal vector $\delta\vec{r}_i$ from the old to new position. The displacement $\delta\vec{r}_i$ is called a virtual displacement which is different from actual displacement $d\vec{r}_i$. Under this change in configuration the system remains in equilibrium indicating that the resultant force acting on each particle of the system is zero, i.e., $\vec{F}_i = 0$, where \vec{F}_i is the force acting on i^{th} particle. Clearly, the virtual work given by $\vec{F}_i \cdot \delta\vec{r}_i$ must be zero.

Thus, $\vec{F}_i \cdot \delta\vec{r}_i = 0$

Summing over all particles, we get

$$\sum_i \vec{F}_i \cdot \delta\vec{r}_i = 0 \quad (1)$$

If the constraints are present, then we write

$$\vec{F}_i = \vec{F}_i^a + \vec{f}_i$$

where \vec{F}_i^a is the actual force and \vec{f}_i is the force of constraints acting on the i^{th} particle. Putting it in equation (1), we get

$$\sum_i (\vec{F}_i^a + \vec{f}_i) \cdot \delta\vec{r}_i = 0$$

or $\sum_i \vec{F}_i^a \cdot \delta\vec{r}_i + \sum_i \vec{f}_i \cdot \delta\vec{r}_i = 0 \quad (2)$

Now restricting ourselves to the system where the virtual work done by the forces of constraints is zero, i.e., $\sum_i \vec{f}_i \cdot \delta\vec{r}_i = 0$ then equation (2) becomes

$$\sum_i \vec{F}_i^a \cdot \delta \vec{r}_i = 0 \quad (3)$$

This is the equation for equilibrium of a system. It states that, a system of particles is in equilibrium only if the total virtual work of the actual applied forces is zero. This is known as principle of virtual work.

6 D'Alembert's principle using virtual work:

D'Alembert's principle is based on the principle of virtual work. Consider a system of finite number of particles. According to Newton's second law of motion, the force on i^{th} particle is defined as

$$\vec{F}_i = \frac{d\vec{P}_i}{dt} = \dot{\vec{P}}_i$$

where \vec{P}_i is the momentum of the i^{th} particle. Thus we have

$$\vec{F}_i - \dot{\vec{P}}_i = 0 \quad (1)$$

According to this equation, a moving system of particles can be considered as in equilibrium under the force $(\vec{F}_i - \dot{\vec{P}}_i)$ where $-\dot{\vec{P}}_i$ is known as reversed effective force on the i^{th} particle.

According to the principle of virtual work, we have

$$\sum_i \vec{F}_i \cdot \delta \vec{r}_i = 0$$

Replacing \vec{F}_i by $(\vec{F}_i - \dot{\vec{P}}_i)$, we get

$$\sum_i (\vec{F}_i - \dot{\vec{P}}_i) \cdot \delta \vec{r}_i = 0 \quad (2)$$

If the forces of constraints are present, then we write

$$\vec{F}_i = \vec{F}_i^a + \vec{f}_i$$

where \vec{F}_i^a is the actual force and \vec{f}_i is the force of constraints acting on the i^{th} particle. Putting it in equation (2), we get

$$\sum_i (\vec{F}_i^a + \vec{f}_i - \dot{\vec{P}}_i) \cdot \delta \vec{r}_i = 0$$

$$\text{or} \quad \sum_i (\vec{F}_i^a - \dot{\vec{P}}_i) \cdot \delta \vec{r}_i + \sum_i \vec{f}_i \cdot \delta \vec{r}_i = 0 \quad (3)$$

By restricting to the systems where the virtual work done by the forces of constraints vanishes, we get

$$\sum_i (\vec{F}_i^a - \dot{\vec{P}}_i) \cdot \delta \vec{r}_i = 0 \quad (4)$$

which is called D'Alembert's principle.

7 Lagrange's equation from D'Alembert's principle:

The coordinate transformation equations are given by

$$\vec{r}_i = \vec{r}_i(q_1, q_2, \dots, q_n, t)$$

where q_1, q_2, \dots, q_n are the generalized coordinates. Differentiating this with respect to time, we get

$$\frac{d\vec{r}_i}{dt} = \frac{\partial \vec{r}_i}{\partial q_1} \frac{dq_1}{dt} + \frac{\partial \vec{r}_i}{\partial q_2} \frac{dq_2}{dt} + \dots + \frac{\partial \vec{r}_i}{\partial q_n} \frac{dq_n}{dt} + \frac{\partial \vec{r}_i}{\partial t} \frac{dt}{dt}$$

$$\text{or} \quad \vec{v}_i = \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \dot{q}_j + \frac{\partial \vec{r}_i}{\partial t} \quad (1)$$

where \vec{v}_i is the velocity of the i^{th} particle. Similarly the virtual displacement $\delta \vec{r}_i$ can be connected with δq_j such as

$$\delta \vec{r}_i = \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j + \frac{\partial \vec{r}_i}{\partial t} \delta t$$

The last term in this equation is zero, since in virtual displacement only coordinate displacement is considered and not that of time. Therefore,

$$\delta \vec{r}_i = \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j \quad (2)$$

D'Alembert's principle is given by

$$\sum_i \left(\vec{F}_i - \dot{\vec{P}}_i \right) \cdot \delta \vec{r}_i = 0 \quad (3)$$

Using equation (2) in it, we get

$$\sum_i \left(\vec{F}_i - \dot{\vec{P}}_i \right) \cdot \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j = 0$$

$$\text{or} \quad \sum_{i,j} \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j - \sum_{i,j} \dot{\vec{P}}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j = 0 \quad (4)$$

$$\text{Let} \quad \sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} = Q_j \quad (5)$$

where Q_j are called components of the generalized force. Thus the equation (4) becomes

$$\sum_j Q_j \delta q_j - \sum_{i,j} \dot{\vec{P}}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j = 0 \quad (6)$$

Further we obtain,

$$\frac{d}{dt} \left(m_i \vec{v}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \right) = m_i \dot{\vec{v}}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} + m_i \vec{v}_i \cdot \frac{d}{dt} \left(\frac{\partial \vec{r}_i}{\partial q_j} \right)$$

$$\text{or} \quad \frac{d}{dt} \left(m_i \vec{v}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \right) = \dot{\vec{P}}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} + m_i \vec{v}_i \cdot \frac{d}{dt} \left(\frac{\partial \vec{r}_i}{\partial q_j} \right)$$

$$\text{or} \quad \dot{\vec{P}}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} = \frac{d}{dt} \left(m_i \vec{v}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \right) - m_i \vec{v}_i \cdot \frac{d}{dt} \left(\frac{\partial \vec{r}_i}{\partial q_j} \right) \quad (7)$$

One can prove the identities

$$\frac{\partial \vec{r}_i}{\partial q_j} = \frac{\partial \vec{v}_i}{\partial \dot{q}_j} \quad \text{and} \quad \frac{d}{dt} \left(\frac{\partial \vec{r}_i}{\partial q_j} \right) = \frac{\partial \vec{v}_i}{\partial q_j}$$

Using these in equation (7), we get

$$\dot{\vec{P}}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} = \frac{d}{dt} \left(m_i \vec{v}_i \cdot \frac{\partial \vec{v}_i}{\partial \dot{q}_j} \right) - m_i \vec{v}_i \cdot \frac{\partial \vec{v}_i}{\partial q_j} \quad (8)$$

Substituting it in equation (6), we have

$$\sum_j Q_j \delta q_j - \sum_{i,j} \left[\frac{d}{dt} \left(m_i \vec{v}_i \cdot \frac{\partial \vec{v}_i}{\partial \dot{q}_j} \right) - m_i \vec{v}_i \cdot \frac{\partial \vec{v}_i}{\partial q_j} \right] \delta q_j = 0$$

$$\text{or} \quad \sum_j Q_j \delta q_j - \sum_j \left[\frac{d}{dt} \left(\frac{\partial}{\partial \dot{q}_j} \left\{ \sum_i \frac{1}{2} m_i v_i^2 \right\} \right) - \frac{\partial}{\partial q_j} \left\{ \sum_i \frac{1}{2} m_i v_i^2 \right\} \right] \delta q_j = 0$$

$$\text{or} \quad \sum_j Q_j \delta q_j - \sum_j \left[\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) - \frac{\partial T}{\partial q_j} \right] \delta q_j = 0 \quad (9)$$

where $\sum_i \frac{1}{2} m_i v_i^2 = T$ is the total kinetic energy of the system.

Rearranging equation (9), we write

$$\sum_j \left[\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) - \frac{\partial T}{\partial q_j} - Q_j \right] \delta q_j = 0$$

As q_j are independent of each other and hence coefficients of δq_j should separately vanish. Therefore,

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) - \frac{\partial T}{\partial q_j} = Q_j \quad (10)$$

Case I :- Conservative system

For conservative system, the forces \vec{F}_i are derivable from potential function V . Thus,

$$\vec{F}_i = -\nabla V_i = -\frac{\partial V}{\partial \vec{r}_i}$$

The generalized force can be expressed as

$$Q_j = \sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} = -\sum_i \frac{\partial V}{\partial \vec{r}_i} \cdot \frac{\partial \vec{r}_i}{\partial q_j} = -\frac{\partial V}{\partial q_j}$$

Substituting it in equation (10), we obtain

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) - \frac{\partial T}{\partial q_j} + \frac{\partial V}{\partial q_j} = 0$$

or
$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) - \frac{\partial (T - V)}{\partial q_j} = 0$$

or
$$\frac{d}{dt} \left(\frac{\partial (T - V)}{\partial \dot{q}_j} \right) - \frac{\partial (T - V)}{\partial q_j} = 0$$

since V is not a function of \dot{q}_j . Therefore,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0$$

where $L = T - V$ is called Lagrangian for the conservative system. Taking summation over j from 1 to n , we get

$$\sum_j \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} \right] = 0 \quad (11)$$

This equation is known as the Lagrangian equation of motion for the conservative system.

Case II :- Non-conservative system

If the system is non-conservative and if the potentials are velocity dependent called generalized potentials, then the equation (9) can be expressed as

$$\sum_j \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} \right] = 0$$

With again $L = T - U$, where $U = U(q_j, \dot{q}_j)$ is the generalized potential.

8 Application of Lagrange's formulation - Simple Pendulum

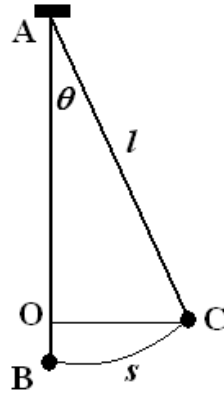


Fig. 1.

Consider a simple pendulum consisting of a bob of mass m suspended to a weightless string of length l as shown in fig 1. Let θ be the angle of displacement then the displacement along arc $OC = s$ is given by

$$s = l\theta \quad (1)$$

The velocity of the bob is

$$v = \frac{ds}{dt} = \frac{d(l\theta)}{dt} = l\dot{\theta} \quad (2)$$

The K. E. is then

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m(l\dot{\theta})^2 \quad (3)$$

Let zero be the potential energy of the system when the bob is at position B.

The P.E. of the system when the bob is at position C is

$$V = mg(OB) = mg(AB - AO) = mg(l - l \cos \theta) = mgl(1 - \cos \theta) \quad (4)$$

Hence,

$$L = T - V = \frac{1}{2}m(l\dot{\theta})^2 - mgl(1 - \cos \theta)$$

Therefore,

$$\frac{\partial L}{\partial \theta} = 0 - mgl(0 + \sin \theta) = -mgl \sin \theta \quad (5)$$

$$\text{and,} \quad \frac{\partial L}{\partial \dot{\theta}} = ml^2 \dot{\theta} \quad (6)$$

Substituting these values in the Lagrangian equation, we get

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\theta}} \right) - \frac{\partial L}{\partial \theta} &= 0 \\ \frac{d}{dt} (ml^2 \dot{\theta}) + mgl \sin \theta &= 0 \\ ml^2 \ddot{\theta} + mgl \sin \theta &= 0 \\ \ddot{\theta} + \frac{g}{l} \sin \theta &= 0 \end{aligned} \quad (7)$$

This represents the equation of motion of a simple pendulum.

For small amplitude oscillations

$$\sin \theta \approx \theta$$

Thus

$$\ddot{\theta} + \frac{g}{l} \theta = 0 \quad (8)$$

This represents a simple harmonic motion of time period given by

$$T = 2\pi \sqrt{\frac{l}{g}} \quad (9)$$

Origin of Quantum Theory

1 Introduction:

The laws of Newtonian mechanics explained successfully the motion of celestial bodies and other earthly objects. These laws along with the laws of thermodynamics and classical electrodynamics explained successfully the physical behavior and bulk properties of matter. However when the same laws were applied to the particles such as electrons, protons, neutrons, nucleus, etc., serious difficulties were encountered. It means that the classical concepts are not valid in the region of atomic dimensions.

In microscopic world of atoms and molecules, the energy and moments were not having the same meaning as in the case of classical dynamics. On the other hand, these dynamic variables had a discrete value in a particular state of an atom and did not undergo change in a continuous manner from one state to another. Thus, to include the new concepts, the Newtonian laws of macroscopic world were modified. This incorporation of new concepts gave rise to the birth of a new mechanics called Quantum Mechanics, which not only explained successfully many observed facts but also introduced revolution in our way of thinking.

It is not to be taken that quantum mechanics does not concern in the macroscopic world. In reality all of physics is quantum physics; the laws of quantum physics are the most general laws of nature.

2 Optical Spectra and Ritz Combination Principle:

Any substance when raised to a high temperature or subjected to an electrical discharge emits light (electromagnetic waves). As a classical view the frequency of the emitted radiations must be equal to mechanical frequency of the electron in its orbit, and to multiples of this as overtones. Due to emission of energy the radius of the orbit would decrease and mechanical energy would change. Consequently the emitted light should have a wide range of wavelengths. This is not in agreement with the experiment because the radiation emitted by hydrogen atom is confined to spectral lines of well-defined frequencies and moreover, these frequencies are not related to one another by integral factors as overtones.

The observed regularities among the spectral lines are expressed by a principle, first formulated by Ritz in 1908, known as Ritz combination principle. According to which a small set of the spectroscopic terms are associated with the atom of the emitting substance such that the wave-numbers means the reciprocal of wavelengths $\bar{\nu} = 1/\lambda$ of various spectral lines are equal to differences between the terms, i.e.,

$$\bar{\nu}_{12} = T_1 - T_2 \quad (1)$$

Neither the spectroscopic terms nor the combination principle could be explained by classical mechanics.

3 Blackbody Radiations:

A perfectly black-body is defined as one, which absorbs all heat radiations incident on it. Experimentally, such a body is represented by a hollow container with a very small aperture in the wall as shown in fig.1a. When a black-body is heated, it emits radiations of all types of wavelengths. These radiations are independent of the nature of the substance. Such heat radiations in a uniform temperature enclosure are known as black-body radiations.

The origin of radiations from a heated body is the rapid vibrating particles composing the body. These particles are called oscillators. According to the classical electrodynamics, these oscillators emit radiant energy in the form of electromagnetic waves. Fig.1b. shows the variation of the intensity of radiation with the wavelength at different temperatures.

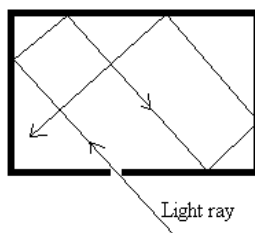


Fig. 1a. Representation of a black body.

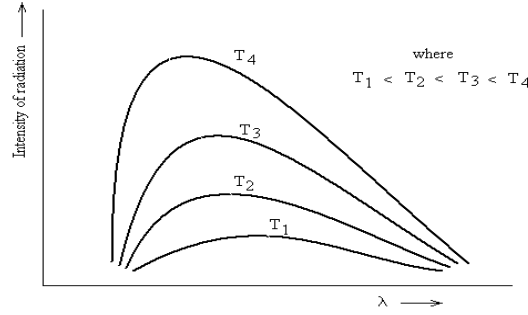


Fig 1b. Variation of intensity of radiation with wavelength at different temperatures.

From fig.1, the following conclusions can be drawn:

- (i) At a given temperature, the energy is not uniformly distributed in the radiation spectrum of a hot body.
- (ii) At a given temperature the intensity of radiations increases with increase in wavelength and at a particular wavelength its value is maximum. With further increase in wavelength, the intensity of heat radiations decreases.
- (iii) With increase in temperature λ_m decreases, where λ_m is the wavelength at which maximum emission of energy takes place.
- (iv) For all wavelengths, an increase in temperature causes an increase in the energy emission.

The area under each curve represents the total energy emitted for the complete spectrum at a particular temperature.

Various attempts were made to construct the shape of the energy spectra as a function of wavelength.

(a) *Wien's contribution:*

Based on the classical electromagnetic theory and assuming that the oscillators from which the radiations are emitted are of molecular size, Wien deduced the expression,

$$E = \frac{a}{\lambda^5} e^{(-b/\lambda T)} \quad (1)$$

where E is energy emitted between wavelengths λ and $\lambda + d\lambda$ and a and b are constants.

It is found that the above equation satisfies the experimental curve in the low wavelength region but do not agree at high wavelength region.

(b) *Rayleigh-Jean's contribution:*

Rayleigh and Jean applied the classical law of equipartition of energy i.e., each vibration mode has an average energy kT to the oscillator of black-body.

Thus,

$$\bar{\epsilon} = kT \quad (2)$$

It was further shown that the number of modes of oscillation dn in the wavelength range λ and $\lambda + d\lambda$ per unit volume of cavity is equal to

$$dn = \frac{8\pi d\lambda}{\lambda^4} \quad (3)$$

The energy density in this wavelength range λ and $\lambda + d\lambda$ equal to $dn\bar{\epsilon}$ and is also equal to $E_\lambda d\lambda$, i.e.,

$$E_\lambda d\lambda = dn\bar{\epsilon}$$

where E_λ is the corresponding energy emitted.

On substituting the values from eq. (2) and from eq. (3) in the above equation we get

$$E_\lambda d\lambda = \left(\frac{8\pi}{\lambda^4} d\lambda \right) kT$$

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

From eq. (4) it follows that E_λ is inversely proportional to the fourth power of wavelength. Thus, E_λ increases with decreasing in λ .

Eq. (4) has been found to fit the experimental data at the high wavelength region but fails completely at the low wavelength region. Thus, Wien's law and Rayleigh-Jean's law based on classical assumptions do not precisely agree with the experimental results.

4 Planck's Radiation Law:

Planck deduced an intermediate expression for blackbody radiation on the basis of the following assumptions:

1. A blackbody radiator contains simple harmonic oscillators of molecular dimensions, which can vibrate with all possible frequencies.
2. The oscillator of the blackbody cannot have any amount of energy but has a discrete energy equal to the integral multiple of some minimum energy, i.e.,

$$\varepsilon = nh\nu \quad (1)$$

where ν is the frequency of an oscillator and n an integer.

3. The oscillators do not radiate or absorb energy continuously. However, the oscillators can exchange energy with its surroundings in discrete values viz. $0, h\nu, 2h\nu, 3h\nu, \dots, nh\nu$, i.e., the multiples of some small unit called the quantum.

Suppose N is the total number of Planck's oscillators and E is their total energy. Then, the energy per oscillator is given as follows:

$$\bar{\varepsilon} = \frac{E}{N} \quad (2a)$$

Let $N_0, N_1, N_2, \dots, N_r, \dots$, etc. be the number of resonators having energy $0, \varepsilon, 2\varepsilon, \dots, r\varepsilon, \dots$, etc. respectively, then we have

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

$$\text{and } E = 0 + \varepsilon N_1 + 2\varepsilon N_2 + \dots + r\varepsilon N_r + \dots$$

$$\text{or } E = \varepsilon(N_1 + 2N_2 + \dots + rN_r + \dots) \quad (2c)$$

According to Maxwell's distribution formula, the number of oscillators having energy $r\varepsilon$ in unit volume will be

$$N_r = N_0 e^{-r\varepsilon/kT}$$

Therefore

$$N_1 = N_0 e^{-\varepsilon/kT}$$

$$N_2 = N_0 e^{-2\varepsilon/kT}$$

.....

Using these in equations (2b) and (2c), we obtain

$$N = N_0 \left(1 + e^{-\varepsilon/kT} + e^{-2\varepsilon/kT} + \dots + e^{-r\varepsilon/kT} + \dots \right)$$

$$\text{or } N = N_0 \left(1 - e^{-\varepsilon/kT} \right)^{-1} = \frac{N_0}{1 - e^{-\varepsilon/kT}} \quad (3)$$

$$\text{and } E = \varepsilon N_0 \left(e^{-\varepsilon/kT} + 2e^{-2\varepsilon/kT} + 3e^{-3\varepsilon/kT} + \dots + re^{-r\varepsilon/kT} + \dots \right)$$

$$E = N_0 \varepsilon e^{-\varepsilon/kT} \left(1 + 2e^{-\varepsilon/kT} + 3e^{-2\varepsilon/kT} + \dots + re^{-\varepsilon(r-1)/kT} + \dots \right)$$

$$\text{or } E = N_0 \varepsilon e^{-\varepsilon/kT} \left(1 - e^{-\varepsilon/kT} \right)^{-2} = \frac{N_0 \varepsilon e^{-\varepsilon/kT}}{\left(1 - e^{-\varepsilon/kT} \right)^2} \quad (4)$$

Substituting these in equation (2), we get

$$\bar{\varepsilon} = \frac{\varepsilon e^{-\varepsilon/kT}}{1 - e^{-\varepsilon/kT}} = \frac{\varepsilon}{e^{\varepsilon/kT} - 1}$$

$$\bar{\varepsilon} = \frac{h\nu}{e^{h\nu/kT} - 1}$$

$$\text{or } \bar{\varepsilon} = \frac{hc/\lambda}{e^{hc/\lambda kT} - 1} \quad (5)$$

Thus we see that average energy of an oscillator is not kT , but given by equation (5).
The number of resonators per unit volume in frequency range λ and $\lambda + d\lambda$ is given by

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

The energy density belonging to range $d\lambda$ can be obtained by multiplying the average energy of an oscillator by the number of resonators per unit volume in the wavelength range λ and $\lambda + d\lambda$, i.e.,

$$E_\lambda d\lambda = \bar{\epsilon}N$$

$$\text{or } E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \times \frac{1}{e^{hc/\lambda kT} - 1} d\lambda \quad (6)$$

This relation is called Planck's radiation law and explains all experimentally observed facts.

Discussion of Result:

1. For small temperatures λT is small. Therefore $e^{hc/\lambda kT} \gg 1$ and 1 in the denominator of equation (6) can be neglected.

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} e^{-hc/\lambda kT} d\lambda$$

which is Wien's Law.

2. For large temperatures λT is large

$$e^{hc/\lambda kT} = 1 + \frac{hc}{\lambda kT} + \left(\frac{hc}{\lambda kT}\right)^2 \frac{1}{2!} + \dots$$

Neglecting higher power terms we have

$$e^{hc/\lambda kT} = 1 + \frac{hc}{\lambda kT}$$

Substituting it in equation (6) we get

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \times \frac{1}{1 + hc/\lambda kT - 1} d\lambda$$

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

This is Rayleigh-Jean's Law.

These results have been verified experimentally, that is, the theoretical values thus calculated agree very well that given by experimental curves.

5 Photoelectric Effect and the laws of photoelectric emission:

Photoelectric effect is the phenomenon of ejections of electrons from a metal plate when light of a suitable wavelength falls on it. It is illustrated in figure 1. The electrons emitted in this process are called photoelectrons and the current produced due to these electrons is called photoelectric current.

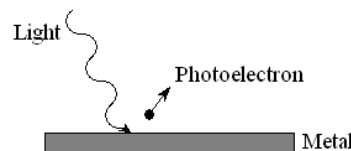


Fig.1. Photoelectric effect.

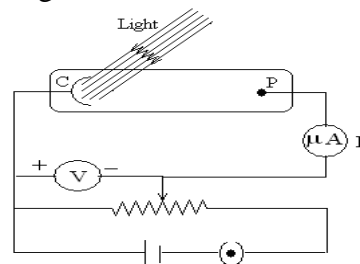


Fig. 2. Experimental arrangement to study photoelectric effect.

The experimental arrangement to study the photoelectric effect is shown in fig. 2. The metal plates P and C are placed in an evacuated glass bulb. The plate C is made up from a photosensitive material. Initially the plate C is connected to the negative terminal and the plate P is connected to the positive terminal of the battery through a micro ammeter. When a specific radiation of fixed frequency and intensity falls on C the photoelectrons are emitted. These photoelectrons, when collected by P kept at positive potential V with respect to plate C, produces a photoelectric current I . If the potential V is increased, the current I gets increased until it reaches a constant value, i.e., it approaches a saturation value as shown in figure 3. If the plate P is made negative with respect to C, the photoelectrons are repelled by P. The photoelectrons whose kinetic energy is greater than eV can reach the plate P. If the plate P is made more and more negative, a stage is reached at which the photoelectric current approaches zero value. This value of potential is called stopping potential V_s . The photoelectrons stopped by V_s have maximum kinetic energy. Let v_{\max} be the maximum velocity of photoelectrons then,

$$\text{Maximum kinetic energy} = \frac{1}{2} m(v_{\max})^2$$

$$\frac{1}{2} m(v_{\max})^2 = eV_s \quad (1)$$

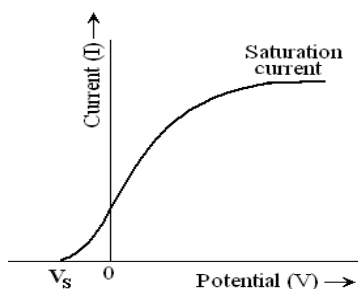


Fig. 3.

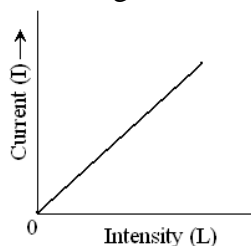


Fig. 4.

For a fixed frequency, the photoelectric current increases linearly with increase in intensity of incident light as shown in fig. 4. The photoelectric current does not depend on frequency of the incident light.

Laws of Photoelectric Effect:

From the experimental facts we state the following characteristics of the photoelectric effect:

- (1) For a given photosensitive surface there is a certain minimum frequency ν_0 of incident radiation, below which there is no emission of photoelectrons. This frequency is called the threshold frequency. The value of threshold frequency ν_0 depends on the material and nature of the emitting surface. There is no emission if the frequency of incident radiation is less than threshold frequency.
- (2) For a given frequency ($\nu > \nu_0$) the number of the photoelectrons emitted per second from a given surface is directly proportional to the intensity of incident radiation. Thus the photoelectric current is directly proportional to the intensity of incident radiation.
- (3) The maximum kinetic energy of the electrons is independent of the intensity of the incident radiation but it is proportional to the frequency of incident radiation.
- (4) The emission of photoelectrons is an instantaneous process. As soon as the radiation of frequency greater than the threshold frequency is incident on a given photosensitive surface, there is emission of photoelectrons.

Classical theory does not give any satisfactory explanation to the photoelectric effect. Einstein successfully explained the photoelectric emission in 1905 on the basis of Planck's quantum theory of radiation. According to the quantum theory, the radiation consists of packets of energy called 'quanta' or

'photons' of energy $h\nu$, where h is the Planck's constant and ν the frequency of radiation. When a photon of energy $h\nu$ is incident upon a metal surface, its energy is used up in two ways:

(a) A part of its energy is used up in ejecting the electron just out of the surface. The energy depends upon the nature of the metal and is called work function W_0 .

(b) The rest part of the energy is used up in imparting kinetic energy $\frac{1}{2}m(v_{\max})^2$ to the ejected electron.

$$\text{Thus } h\nu = W_0 + \frac{1}{2}m(v_{\max})^2 \quad (2)$$

$$\text{But } h\nu_0 = W_0$$

where ν_0 is the threshold frequency. Therefore, equation (2) becomes

$$h\nu = h\nu_0 + \frac{1}{2}m(v_{\max})^2 \quad (3)$$

This equation is called Einstein's photoelectric equation, which successfully explains all the characteristics of the photoelectric effect.

Q. Show how the classical theory was failed to explain the Photoelectric Effect.

Ans. Photoelectric effect is the phenomenon of ejections of electrons from a metal surface when light of a suitable wavelength falls on it. The electrons emitted in this process are called photoelectrons.

Classical theory (electromagnetic theory) was first used to explain the photoelectric effect. According to this theory the electric exerts forces on the electrons and so there is emission of electrons from the surface. However the classical theory fails to explain the photoelectric effect in the following respects.

1. Instantaneous emission of photoelectrons: According to the classical the energy transmitted by the light is smoothly and equally distributed through the space. Each electron would get a very small amount of energy of it and if this energy is not enough in comparison with the binding energy then the electron would accumulate the energy with time and after getting sufficient energy in few times it would escape from the metal surface. So the classical theory does not support to the instantaneous emission.

2. Threshold frequency, ν_0 : The classical theory is unable to explain why the photoelectrons are not emitted from the metal surface when the light radiation has a frequency less than the threshold frequency though the intensity is very high, whereas, the very low intensity and high frequency radiations can produce the photoelectrons.

3. Proportionality of the kinetic energy of the photoelectrons with the frequency of the incident radiation: The classical theory expects that the kinetic energy of the photoelectrons should be proportional to the intensity of the incident radiation, whereas, the experimental results indicate that it is proportional to the frequency of the incident radiation.

Thus the classical theory fails to explain the photoelectric effect.

Q. Write short note on Einstein's explanation of Photoelectric Effect.

Ans: Photoelectric effect is the phenomenon of ejections of electrons from a metal surface when light of a suitable wavelength falls on it. The electrons emitted in this process are called photoelectrons.

Classical theory (electromagnetic theory) was first used to explain the photoelectric effect. According to this theory the electric and magnetic fields associated with the light wave exerts forces on the electrons and so there is emission of electrons from the surface. However the classical theory fails to explain the photoelectric effect in all respects.

As the classical theory failed to explain the photoelectric effect, Einstein explained it by using the Plank's quantum concept in 1905. He assumed that the energy of the light is not continuously distributed over the whole expanding wave front but is concentrated into the small regions in terms of packets. Each of these packets have energy $h\nu$, where ν is the frequency of the light wave and h is the plank's constant. Each of these packets is called as **photons**. Thus when the light radiation of frequency ν is incident on the

metal surface, the electron absorbs the energy $h\nu$ of the photon. Part of this energy is used by the electron in escaping from the metal surface and remaining appears as kinetic energy of photoelectron. If the photoelectron does not lose any part of this energy in collision inside the metal surface, it escapes with maximum kinetic energy. Thus the energy of the photon is the sum of the maximum kinetic energy of the photoelectron and the energy required to release the photoelectron from the metal surface. Let v_{\max} be the maximum velocity of the photoelectron then we have,

$$h\nu = \frac{1}{2} v_{\max}^2 + W_0 \quad (1)$$

where W_0 represents the maximum energy required for the electron to release from the metal surface and is called as the photoelectric work function for the given metal surface.

Equation (1) is called Einstein's photoelectric equation. Clearly this equation shows that, As W_0 is constant for a given metal surface, the kinetic energy of the photoelectron is directly proportional to the frequency of the incident radiation.

If the frequency of the incident photon is gradually decreased, the kinetic energy of the photoelectron becomes less and less, reaching zero at a value ν_0 called the threshold frequency, giving $h\nu_0 = W_0$. Then the Einstein's equation takes the form

$$\frac{1}{2} v_{\max}^2 = h\nu - h\nu_0 = h(\nu - \nu_0)$$

When $\nu > \nu_0$, the kinetic energy is positive and the photoelectrons are emitted. In case $\nu < \nu_0$, kinetic energy is negative and there is no emission of the photoelectrons.

iii. The velocity of the photoelectrons is independent of the intensity of radiation. By keeping ν constant, the increase in intensity of radiation would merely increase the number of photons striking the metal surface, which causes to increase the number of photoelectrons or the photocurrent.

iv. There is no time lag in this process. For this phenomenon it is conceived that there is collision between photon and the electron the result of the collision is always instantaneous. Hence the photoelectric effect is instantaneous.

Thus each and every characteristic of the photoelectric effect receives an adequate interpretation on principle of quantum theory.

De Broglie's Wave and Uncertainty Principle

1 Inadequacy of classical mechanics

1.1 Stability of the atom:

Experiments of Rutherford (1910) had established that an atom consisted of a heavy positively charged nucleus surrounded by negatively charged electrons of very little mass. If the classical picture is adopted according to Earnshaw, the system will be stable only if the negatively charged electrons are kept revolving around the positively charged heavy nucleus in a similar manner as the planets are revolving around the sun. But unlike the planets, the energy of the moving electrons should decrease because the accelerated charged particle such as electron radiates out energy continuously in the form of electromagnetic waves. Therefore, due to this continuous loss of energy an orbiting electron will come closer and closer to the nucleus and ultimately will fall in the nucleus. This shows the instability of the atom i.e., it is in contradiction to the observed fact of the stability of the atom. Thus, the classical mechanics fails to explain the stability of the atom.

1.2 Spectrum of the hydrogen atom:

The classical mechanics did not explain the spectrum of the hydrogen atom. Experimentally it was observed that the hydrogen spectrum consists of a discrete set of lines represented by

$$\bar{\nu} = R \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Where $\bar{\nu}$ is the wave number and n_1 and n_2 are integers such that $n_1 < n_2$.

According to the classical theory the excited atoms of hydrogen emit electromagnetic radiations of all wavelengths continually, while they emit the radiations of certain wavelengths only. This difficulty was further resolved by Bohr up to some extent.

From the above discussion it can be concluded that the classical mechanics does not hold good in the region of atomic dimensions.

2 Two slit experiment

The experimental arrangement of two slit experiment is as shown in fig 1. The electron gun supplies the electrons of known velocity in the form of a fine electron beam. The velocity of the electron is known from the accelerating potential. The electrons emerging from the gun are allowed to pass through the two slits S_1 and S_2 . The interference pattern is observed on the photographic plate film P . The entire apparatus is enclosed in a high vacuum chamber, so that electrons emerging from the gun travel to the screen without collision in the path. When the photographic film is observed with an electron microscope, it is observed that interference fringes are found on the film. The distribution of the intensity on the film is shown on the right in the figure. The formation of the interference fringes clearly indicates the wave nature of the electrons.

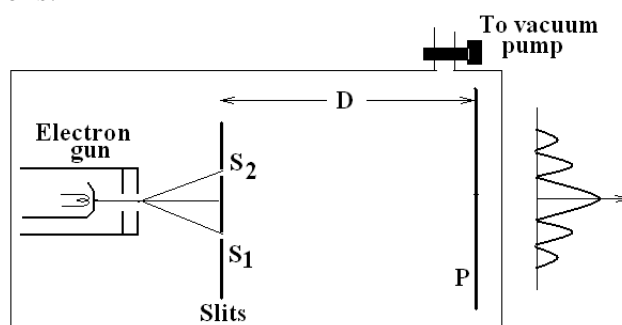


Fig. 1.

If V is the accelerating potential given to the final accelerating anode in the electron gun then
 $K. E. = P. E.$

$$\text{or } \frac{1}{2} m v^2 = eV$$

$$\text{or } \frac{m^2 v^2}{2m} = eV$$

$$\text{or } \frac{p^2}{2m} = eV$$

$$\text{or } p = \sqrt{2meV}$$

(1)

According to de Broglie hypothesis, the wavelength of the electron is

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

Using equation (1), we get

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

Thus the wavelength of the electron can be obtained.

Further when two waves interact, the principle of superposition says that the resulting wave function is the sum of the two individual wave functions. This phenomenon is generally described as interference. Here interference fringes are formed because of the electrons are behaving as waves. According to the two-slit experiment, the wavelength of the monochromatic light involved in the experiment is given by

$$\lambda = \frac{xL}{D} \quad (3)$$

Where x is the distance between two consecutive minima or maxima (fringes) on the film, D is the distance of the screen from the slits and L is the distance between the slits.

It is found that the wavelengths given by equations (2) and (3) are found to be same which confirms the de Broglie's hypothesis.

3 de Broglie's Hypothesis: Matter Waves

We know that up to 1926 the matter particles were considered to be completely in nature. But in that year de Broglie proposed that a material particle such as an electron, proton etc., might have a nature like just light wave. i.e., a matter can have dual nature-particle nature as well as wave nature and is called as de Broglie's hypothesis.

A photon of light of frequency ν has the momentum

$$p = \frac{h\nu}{c}$$

or
$$p = \frac{h}{\lambda} \quad (1)$$

since $\lambda = c/\nu$

The wavelength of a photon is, therefore,

$$\lambda = \frac{h}{p} \quad (2)$$

de Broglie considered that equation (2) is a general formula and can be applied to material particles as well as photons. The momentum of a particle of mass m and velocity v is

$$p = mv$$

and consequently its de Broglie wavelength is

$$\lambda = \frac{h}{mv} \quad (3)$$

Equation (3) gives de Broglie wavelength of a particle having mass m moving with velocity v . If the velocity of the particle is comparable to the velocity of light c then the following relativistic formula for mass is to be used.

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

where m_0 is the rest mass of the particle.

4 De Broglie model of the atom:

In 1924, a French physicist named Louis de Broglie suggested that, like light, electrons could act as both particles and waves. De Broglie's hypothesis was soon confirmed in experiments that showed electron beams could be diffracted or bent as they passed through a slit much like light could. So, the waves produced by an electron confined in its orbit about the nucleus sets up a standing wave of specific wavelength, energy and frequency as shown in figure 1(a).

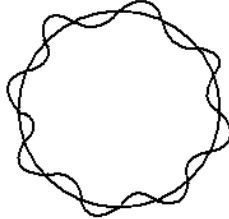


Fig. 1(a). Wave in phase.

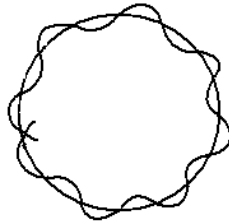


Fig. 1(b). Wave out of phase.

For the wave to remain continuously in phase, the circumference of the orbit should be integral multiple of wave length λ , i.e.,

$$2\pi r = n\lambda \quad (1)$$

Where r is the radius of the orbit and n is the whole number.

We know

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

Substituting the value of λ in equation (1), we get

$$2\pi r = n \frac{h}{mv}$$

$$\text{or } mvr = n \frac{h}{2\pi} \quad (2)$$

which is the same as the Bohr's second postulate. From equation (2), it follows that "Electron can move only in such orbits for which the angular momentum must be the integral multiple of $h/2\pi$." If the circumference is bigger or smaller than the value given by equation (2), it means that the wave is not in phase as shown in figure 1(b). Thus de Broglie relation provides a theoretical base for the Bohr's second postulate.

5 The Concept of Wave and Group Velocities:

According to de-Broglie hypothesis a material particle in motion has a wave of wavelength $\lambda = \frac{h}{mv}$ associated with it, where m is the mass of the particle and v is its velocity. If E is the energy of the particle, then the frequency ν of the wave can be specified by the quantum condition $E = h\nu$, thereby giving $\nu = E/h$. But according to Einstein's mass energy relation $E = mc^2$, so that

$$\nu = mc^2/h \quad (a)$$

The de-Broglie wave velocity w is given by

$$w = \lambda\nu = \frac{mc^2}{h} \frac{h}{mv}$$

$$\text{or } w = \frac{c^2}{v} \quad (b)$$

According to Einstein's theory relativity, the speed of light is maximum velocity that can be attained by a particle in nature, i.e., the velocity of material particle 'v' is always less than the speed of light 'c'. Accordingly equation (b) implies that the de-Broglie wave velocity w must be greater than c. This is an unexpected result. Furthermore according to this result, the de-Broglie wave associated with the particle would travel faster than the particle itself, thus leaving the particle far behind. Thus it is clear that a material particle cannot be equivalent to a single wave train.

The difficulty was resolved by Schrödinger by postulating that a material particle in motion is equivalent to a wave packet rather than a single wave. A wave packet comprises a group of waves, each with slightly different velocity and wavelength, with phases and amplitudes so chosen that they interfere constructively over only a small region of space where the particle can be located, outside of which they produce destructive interference so that the amplitude reduces to zero rapidly. The amplitude of one dimensional wave packet, in general, resembles to curve of fig. 1. Such a wave packet moves with its own velocity called group velocity. The individual wave forming the packet possesses an average velocity, called the phase velocity. It can be shown that the velocity of the material particle v is same as group velocity of the group of wave.

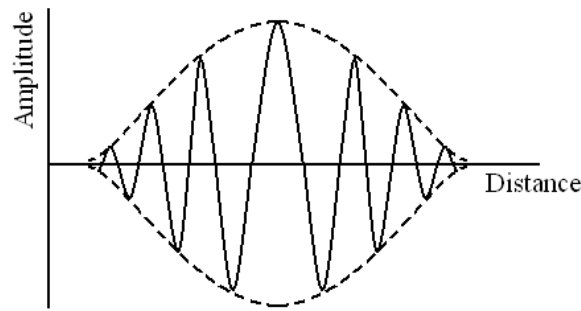


Fig.1. Representation of a wave packet.

Let us assume that the two wave-trains have the same amplitude; but slightly different frequencies and phase velocities such that they can be represented by the equations

$$y_1 = A \cos(\omega t - kx) \quad (1)$$

$$y_2 = A \cos[(\omega + d\omega)t - (k + dk)x] \quad (2)$$

The resultant amplitude of the wave may be obtained by adding (1) and (2), i.e.,

$$y = y_1 + y_2 = A \{ \cos(\omega t - kx) + \cos[(\omega + d\omega)t - (k + dk)x] \}$$

Using $\cos \alpha + \cos \beta = 2 \cos\left(\frac{\alpha + \beta}{2}\right) \cos\left(\frac{\alpha - \beta}{2}\right)$

we get

$$y = 2A \cos\left(\frac{[2\omega + d\omega]t - [2k + dk]x}{2}\right) \cos\left(\frac{d\omega t - dkx}{2}\right)$$

Since $d\omega$ and dk are small compared with ω and k respectively, we have

$$2\omega + d\omega \approx 2\omega \quad \text{and} \quad 2k + dk \approx 2k$$

Therefore,

$$y = 2A \cos(\omega t - kx) \cos\left(\frac{d\omega}{2} t - \frac{dk}{2} x\right) \quad (3)$$

Equation (3) represents a wave of angular frequency ω and propagation constant k that has superimposed upon it by a modulation of angular frequency $d\omega/2$ and a propagation constant $dk/2$. The effect of the modulation is to produce successive wave groups as shown in fig.1. The wave velocity w is given by

$$w = \omega/k \quad (4)$$

while the velocity u of the wave group or the group velocity u is

$$u = d\omega/dk \quad (5)$$

The angular frequency and the propagation constant of the de Broglie waves associated with a body of rest mass m_0 moving with velocity v are

$$\omega = 2\pi\nu = 2\pi\frac{h\nu}{h} = 2\pi\frac{E}{h} = 2\pi\frac{mc^2}{h} = \frac{2\pi m_0 c^2}{h\sqrt{1-\frac{v^2}{c^2}}} \quad (6)$$

and

$$k = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h} = \frac{2\pi m_0 v}{h\sqrt{1-\frac{v^2}{c^2}}} \quad (7)$$

The wave velocity w is as we found earlier,

$$w = \omega/k = c^2/v$$

which exceeds the velocity of light c .

The group velocity u of the de Broglie waves associated with body is

$$u = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv} \quad (8)$$

Differentiating equations (6) and (7) with respect to v we get

$$\frac{d\omega}{dv} = \frac{2\pi m_0 v}{h\left(1-\frac{v^2}{c^2}\right)^{3/2}} \quad (9)$$

$$\text{and} \quad \frac{dk}{dv} = \frac{2\pi m_0}{h\left(1-\frac{v^2}{c^2}\right)^{3/2}} \quad (10)$$

Therefore, the group velocity is

$$u = v \quad (11)$$

Thus the de Broglie wave group associated with a moving body travels with the same velocity as the body.

6 Heisenberg's Uncertainty Principle:

It states that the product of uncertainty Δx in determining the position of particle at some instant and the uncertainty Δp in momentum of the particle at the same instant is equal to or greater than $\hbar (= h/2\pi)$.

i.e.,

$$\Delta x \Delta p = \hbar \quad (1)$$

Werner Heisenberg in 1927 stated such relationship in the form of principle called 'Uncertainty Principle' as given by equation (1). We know that a moving body is always associated with de Broglie waves; further interference of these waves causes a wave group formation. This clearly suggests that there is a fundamental limit to the accuracy with which particle properties can be measured. If the wave group representing the particle is very narrow as shown in Fig 1 (a), the position of the particle is certain but the determination of wavelength and hence the momentum (since $\lambda=h/p$) becomes uncertain. On the other hand, if the wave group is wide as in Fig. 1 (c), accurate determination of wavelength and hence the momentum is possible but the position determination of particle within the wave group becomes uncertain.



Fig. 1a.

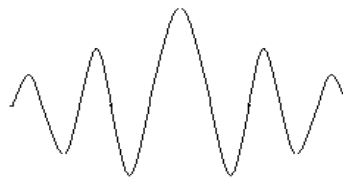


Fig. 1b.

The simplest example of the formation of wave groups is that the superposition of two wave trains slightly different in angular frequency ω and propagation constant k . Consider such de Broglie waves with amplitude A . Let

$$\psi_1 = A\cos(\omega t - kx) \quad (2)$$

$$\psi_2 = A\cos[(\omega + \Delta\omega)t - (k + \Delta k)x] \quad (3)$$

The resultant wave group is then

$$\begin{aligned} \Psi &= \psi_1 + \psi_2 \\ \Psi &= 2A\cos(\omega t - kx)\cos[(\Delta\omega/2)t - (\Delta k/2)x] \end{aligned} \quad (4)$$

This is plotted in the Fig 2. The width of each group is evidently equal to half the wavelength λ_m of the modulation.

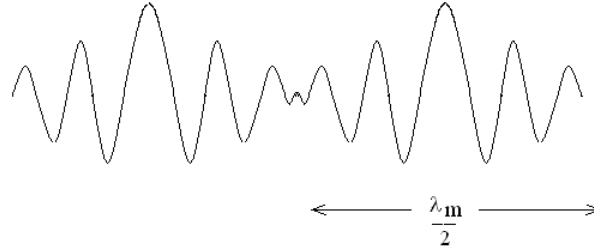


Fig. 2.

It can be suppose that this width is of the same order of magnitude as the inherent uncertainty Δx in the position of the particle, that is

$$\Delta x = \frac{1}{2}(\lambda_m) \quad (5)$$

The modulation wavelength λ_m is related to its propagation constant k_m by

$$\lambda_m = 2\pi/k_m$$

From equation (4), the propagation constant k_m is

$$k_m = \Delta k/2$$

Therefore,

$$\lambda_m = \frac{2\pi}{\Delta k/2}$$

Substituting it in equation (5), we get

$$\Delta x = \frac{1}{2} \frac{2\pi}{\Delta k/2}$$

$$\text{or } \Delta x = \frac{2\pi}{\Delta k} \quad (6)$$

The de Broglie wavelength of a particle of momentum p is

$$\lambda = h/p$$

The propagation constant corresponding to this wavelength is

$$k = 2\pi/\lambda$$

Substituting it in above equation, we get

$$k = (2\pi p)/h$$

Hence an uncertainty Δk in the propagation constant of the de Broglie waves associated with the particle results in an uncertainty Δp in the particle's momentum according to the formula

$$\Delta k = (2\pi\Delta p)/h \quad (7)$$

Substituting the value of Δk in equation (6), we obtain

$$\Delta x = \frac{2\pi h}{2\pi\Delta p}$$

$$\begin{aligned} \text{or } \Delta x\Delta p &= h \\ \Delta x\Delta p &\geq h \end{aligned} \quad (8)$$

The sign \geq is due to the fact that wave groups may have different shapes. Thus, in equation (8), Δx . and Δp are irreducible minima, which are consequences of the wave nature of moving bodies. More convenient form of uncertainty relation being used is

$$\Delta x \Delta p \geq \hbar \quad (9)$$

The time-energy Uncertainty Principle:

Another form of the uncertainty principle is sometimes useful. Suppose we wish to measure the energy E emitted sometime during the time interval Δt in an atomic process. If the energy is in the form of electromagnetic waves, the limited time available restricts the accuracy with which we can determine the frequency ν of the waves. Since the frequency is the reciprocal of time period, the uncertainty $\Delta \nu$ in our frequency measurement is

$$\Delta \nu = 1/(\Delta t) \quad (10)$$

The corresponding energy uncertainty is

$$\Delta E = h \Delta \nu$$

Using equation (10), we have

$$\Delta E = h/(\Delta t)$$

or $\Delta E \Delta t = h$

A more realistic calculation changes above equation to

$$\Delta E \Delta t \geq \hbar \quad (11)$$

This equation states that the product of the uncertainty ΔE in an energy measurement at any instant and the uncertainty Δt in the time measured at the same instant is equal to or greater than \hbar .

7 Application of uncertainty principle: Energy and radius of Bohr's orbit

The energy of an electron in hydrogen atom is given by

$$E = K.E. + P.E. = \frac{p^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 r} \quad (1)$$

where

p – momentum of the electron,

m – mass of the electron,

Z – atomic number,

e – charge on electron,

ϵ_0 – free space permeability,

r – radius of the orbit.

The uncertainty ΔE in the total energy of the electron is then

$$\Delta E = \frac{(\Delta p)^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 \Delta x} \quad (2)$$

where Δp and Δx are the corresponding uncertainties in the momentum and position of the electron.

The Heisenberg's uncertainty relation is

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

or
$$\Delta p = \frac{\hbar}{\Delta x} = \frac{h}{2\pi\Delta x}$$

Substituting it in equation (2), we get

$$\Delta E = \frac{h^2}{8\pi^2 m (\Delta x)^2} - \frac{Ze^2}{4\pi\epsilon_0 \Delta x} \quad (3)$$

The uncertainty in the energy will be minimum if

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

Differentiating equation (3) with respect Δx . we get

$$\frac{d(\Delta E)}{d(\Delta x)} = \frac{-2h^2}{8\pi^2 m (\Delta x)^3} + \frac{Ze^2}{4\pi\epsilon_0 (\Delta x)^2} \quad (4)$$

or
$$0 = \frac{-2h^2}{8\pi^2 m (\Delta x)^3} + \frac{Ze^2}{4\pi\epsilon_0 (\Delta x)^2}$$

$$\text{or } \Delta x = \frac{\epsilon_0 h^2}{\pi m Z e^2} \quad (5)$$

Differentiating equation (4) with respect Δx . we get

$$\frac{d^2(\Delta E)}{d(\Delta x)^2} = \frac{3h^2}{4\pi^2 m (\Delta x)^4} - \frac{Ze^2}{2\pi\epsilon_0 (\Delta x)^3}$$

$$\text{or } \frac{d^2(\Delta E)}{d(\Delta x)^2} = \frac{3h^2}{4\pi^2 m (\Delta x)^3 (\Delta x)} - \frac{Ze^2}{2\pi\epsilon_0 (\Delta x)^3}$$

$$\text{or } \frac{d^2(\Delta E)}{d(\Delta x)^2} = \frac{3h^2}{4\pi^2 m (\Delta x)^3} \frac{\epsilon_0 h^2}{\pi m Z e^2} - \frac{Ze^2}{2\pi\epsilon_0 (\Delta x)^3}$$

$$\text{or } \frac{d^2(\Delta E)}{d(\Delta x)^2} = \frac{Ze^2}{2\pi\epsilon_0 (\Delta x)^3} \left[\frac{3}{2} - 1 \right]$$

$$\text{or } \frac{d^2(\Delta E)}{d(\Delta x)^2} = \frac{Ze^2}{4\pi\epsilon_0 (\Delta x)^3} = +ve$$

The equation (5) is the condition for minimum energy. Therefore, the radius of the first Bohr's orbit would be

$$r = \frac{\epsilon_0 h^2}{\pi m Z e^2} \quad (6)$$

For electron to revolve in a circular orbit we must have the centrifugal force equal to the centripetal force. Thus

$$\frac{mv^2}{r} = \frac{Ze^2}{4\pi\epsilon_0 r^2}$$

$$\text{or } \frac{m^2 v^2}{m} = \frac{Ze^2}{4\pi\epsilon_0 r}$$

$$\text{or } \frac{p^2}{m} = \frac{Ze^2}{4\pi\epsilon_0 r}$$

Substituting it in the equation (1), we get the total energy of the electron in first orbit as

$$E = \frac{Ze^2}{8\pi\epsilon_0 r} - \frac{Ze^2}{4\pi\epsilon_0 r} = -\frac{Ze^2}{8\pi\epsilon_0 r}$$

Substituting the value of r from equation (6), we get

$$E = -\frac{Ze^2}{8\pi\epsilon_0 \frac{\epsilon_0 h^2}{\pi m Z e^2}}$$

$$\text{or } E = -\frac{m Z^2 e^4}{8\epsilon_0^2 h^2} \quad (7)$$

This is the energy of the electron in the Bohr's first orbit of the hydrogen atom.

8 Application of uncertainty principle: Electron cannot present in the nucleus

The radius of typical nuclei is of the order 10^{-14} m. If an electron to be present in the nucleus the uncertainty in its position must be greater than or equal to the radius of the nucleus. Therefore, the minimum uncertainty in its position should be 2×10^{-14} m. Thus

$$\Delta x \approx 2 \times 10^{-14} \text{ m}$$

According to Heisenberg's uncertainty principle,

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

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

$$\text{or } \Delta p \approx \frac{1.055 \times 10^{-34}}{2 \times 10^{-14}} = 5.275 \times 10^{-21} \text{ kg.m/sec} \quad (1)$$

if this is the uncertainty in the momentum of the electron then the corresponding momentum of the electron must be at least comparable with this magnitude, i.e.,

$$p \approx 5.275 \times 10^{-21} \text{ kg.m/sec} \quad (2)$$

The kinetic energy of the electron of mass m is given by

$$T = \frac{p^2}{2m}$$

$$\text{or } T = \frac{(5.275 \times 10^{-21})^2}{2 \times 9.1 \times 10^{-31}} \text{ joule}$$

$$\text{or } T = \frac{(5.275 \times 10^{-21})^2}{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}} \text{ eV}$$

$$\text{or } T = 9.7 \times 10^7 \text{ eV}$$

$$\text{or } T = 97 \text{ MeV}$$

This means that if an electron to be present in the nucleus, its kinetic energy must be of the order of 97 MeV. But experimental observations show that no electron in the atom possesses energy greater than 4 MeV. Clearly it indicates that the electrons do not exist in the nucleus.

Schrodinger's Equation

1 Wave function (ψ):

According to the de-Broglie hypothesis a particle in motion is always associated with a wave represented by a function ψ . Though the wave function ψ itself has no physical significance, the square of its absolute magnitude $|\psi|^2$ (or $\psi^*\psi$ if ψ is a complex) evaluated at a particular time at a particular point is proportional to the probability of finding the particle at that time.

Thus if

$$\int_{-\infty}^{\infty} |\psi|^2 dv = \text{finite} \quad (1)$$

then the particle exists somewhere in the space.

If

$$\int_{-\infty}^{\infty} |\psi|^2 dv = 0 \quad (2)$$

then the particle does not exist in the space.

If

$$\int_{-\infty}^{\infty} |\psi|^2 dv = \infty \quad (3)$$

then the particle exists everywhere simultaneously in the space which is not acceptable.

Now it is convenient to use $|\psi|^2$ equal to the probability p of finding the particle described by ψ rather than merely be proportional to p . Thus if

$$|\psi|^2 = p \quad \text{then}$$

$$\int_{-\infty}^{\infty} |\psi|^2 dv = 1 \quad (4)$$

Since $\int_{-\infty}^{\infty} p dv = 1$

It implies that the particle exists somewhere at all times. A wave function which obeys the equation (4) is said to be normalized wave function. It may be noted that every acceptable wave function can be normalized by multiplying it with an appropriate constant. In addition to the normalization the wave function ψ must be single valued, since p can have only one value at a particular place and time. Further the wave function ψ and its partial derivatives $\frac{\partial \psi}{\partial x}$, $\frac{\partial \psi}{\partial y}$, $\frac{\partial \psi}{\partial z}$ must be continuous everywhere.

2 Schrödinger's equation: Time-dependent form

According to de Broglie hypothesis, a particle in motion is always associated with a wave function ψ , which itself is a complex quantity. Its equation can be written as

$$\psi = Ae^{-i\omega\left(t - \frac{x}{v}\right)} \quad (1)$$

This equation can be converted to present the particle properties as follows.

If ν is the frequency of the wave then the angular frequency is $\omega = 2\pi\nu$ and also the velocity v of the wave is given by $v = \nu\lambda$.

Therefore,
$$\omega\left(t - \frac{x}{v}\right) = 2\pi\nu\left(t - \frac{x}{v\lambda}\right) = \frac{2\pi}{h}h\nu\left(t - \frac{x}{v\lambda}\right) = \frac{2\pi}{h}\left(h\nu t - \frac{h\nu x}{\lambda}\right) = \frac{2\pi}{h}(Et - px)$$

or
$$\omega\left(t - \frac{x}{v}\right) = \frac{1}{\hbar}(Et - px)$$

Substituting it in equation (1), we get

$$\psi = Ae^{-\frac{i}{\hbar}(Et - px)} \quad (2)$$

This is the wave associated with a freely moving particle of total energy E and momentum p moving in the positive direction of x -axis. To obtain Schrodinger's equation, let us differentiate twice equation (2) with respect x , we get

$$\frac{\partial \psi}{\partial x} = \frac{\partial}{\partial x} \left(Ae^{-\frac{i}{\hbar}(Et - px)} \right) = \left(Ae^{-\frac{i}{\hbar}(Et - px)} \right) \left(-\frac{i}{\hbar} \right) (-p)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \left(Ae^{-\frac{i}{\hbar}(Et - px)} \right) \left(-\frac{i}{\hbar} \right) (-p) \left(-\frac{i}{\hbar} \right) (-p)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \left(Ae^{-\frac{i}{\hbar}(Et - px)} \right) \left(\frac{ip}{\hbar} \right) \left(\frac{ip}{\hbar} \right)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \left(Ae^{-\frac{i}{\hbar}(Et - px)} \right) \left(-\frac{p^2}{\hbar^2} \right)$$

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

$$\text{or} \quad \frac{p^2}{2m} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad (3)$$

Similarly, differentiating equation (2) with respect t , we get

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

$$\text{or} \quad E\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (4)$$

If the particle speed is small as compared to the speed of light, the total energy of the particle is give by

$$\text{Total energy} = \text{K.E.} + \text{P.E.}$$

$$E = (1/2)mv^2 + V$$

$$E = (p^2/2m) + V$$

Multiplying by the wave function, we get

$$E\psi = (p^2/2m)\psi + V\psi \quad (5)$$

Using the equations (3) and (4) in equation (5), we get

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \quad (6)$$

The equation (6) is called the time-dependent form of Schrödinger's equation. In three it becomes

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

$$\text{or} \quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \quad (7)$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is called Laplacian operator. The potential function V is a function of position and time.

3 Expectation Values:

By setting up a Schrödinger's equation for a particle in a given situation all the information regarding the particle can be obtained by knowing the wave function $\psi(x, t)$ associated with it. Such a wave function is obtained by solving the Schrödinger's equation. This information is in general in the form of probabilities and not in the form of definite figures. It is due to uncertainties in measurements. Therefore, in quantum mechanics the information is obtained in terms of expectation values. Suppose we wish to obtain the expectation value x of the position of a particle described by the wave function $\psi(x, t)$.

For that, usually positions of a number of particles described by same wave function ψ at some instant are determined experimentally and then are averaged to get \bar{x} . Further, considering the case of many particles distributed at different positions along x-axis. We find average or mean positions along x-axis of all particles. If N_1 number of particles is at x_1 , N_2 number of particles is at x_2 and so on, then the average position \bar{x} in this case is similar to the centre of mass of the distribution

i.e.
$$\bar{x} = \frac{N_1x_1 + N_2x_2 + N_3x_3 + \dots}{N_1 + N_2 + N_3 + \dots}$$

or
$$\bar{x} = \frac{\sum_{i=1}^n N_i x_i}{\sum_{i=1}^n N_i} \tag{1}$$

Quantum mechanically, this expression can be modified for a single particle, by replacing the number N_i of particles at x_i by the probability P_i . The probability that the particle may be found in an interval dx at x_i may be given as

$$P_i = |\psi_i|^2 dx \tag{2}$$

where ψ_i is wave function associated with the particle. Substituting (2) in (1) and taking integral between limits $-\infty$ to $+\infty$ instead of the summation, we have

$$\bar{x} = \frac{\int_{-\infty}^{\infty} x |\psi|^2 dx}{\int_{-\infty}^{\infty} |\psi|^2 dx} \tag{3}$$

If the wave function is normalized, then

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

Thus, equation (3) becomes

$$\bar{x} = \int_{-\infty}^{\infty} x |\psi|^2 dx \tag{4}$$

The equation (4) is more conveniently written as

$$\bar{x} = \int_{-\infty}^{\infty} \psi^* x \psi dx \tag{5}$$

where ψ^* is complex conjugate of ψ .

The expectation value $G(x)$ of any quantity which is a function of the position x of a particle and is described by a wave function ψ may be expressed as

$$\bar{G} = \int_{-\infty}^{\infty} \psi^* G(x) \psi dx \tag{6}$$

The expression (6) holds even if $G(x)$ changes with time, since ψ is function of time t .

4 Operators:

The expectation values of momentum P and energy E of a particle describing by a wave function ψ is given by

$$\bar{p} = \int_{-\infty}^{\infty} \psi^* p \psi dx \tag{1}$$

$$\bar{E} = \int_{-\infty}^{\infty} \psi^* E \psi dx \tag{2}$$

where P and E must be functions of x and t in order to carry out integration in (1) and (2). This is required because $\psi = \psi(x, t)$. However, the uncertainty principle does not allow such dependence of p and E on x

and t , which in turn introduces an error in determination of P and E . Therefore, instead of eqns (1) and (2), other expressions are required to calculate expectation values of momentum and energy respectively. Quantum mechanically it is suggested that the expectation values of P and E may be obtained by differentiating the wave function representing the free particle. Now,

$$\psi = Ae^{-\frac{i}{\hbar}(Et - px)} \quad (3)$$

Differentiating the above equation w.r.t. x and t we get

$$\frac{\partial \psi}{\partial x} = \frac{\partial}{\partial x} \left(Ae^{-\frac{i}{\hbar}(Et - px)} \right) = \left(Ae^{-\frac{i}{\hbar}(Et - px)} \right) \left(-\frac{i}{\hbar} \right) (-p)$$

$$\frac{\partial \psi}{\partial x} = \frac{i}{\hbar} p \psi$$

and

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

Rearranging these equations, we get

$$p \psi = -i\hbar \frac{\partial}{\partial x} \psi \quad (4)$$

and

$$E \psi = i\hbar \frac{\partial}{\partial t} \psi \quad (5)$$

Thus the momentum P and total energy E , that are dynamical quantities, correspond to the differential operators namely $-i\hbar \frac{\partial}{\partial x}$ and $i\hbar \frac{\partial}{\partial t}$ respectively. So, denoting momentum and energy operators by \hat{p} and \hat{E} respectively, we write

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \quad (6)$$

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \quad (7)$$

The kinetic energy operator can be obtained as

$$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \quad (8)$$

The expectation values of momentum and energy are, then, obtained as

$$\bar{p} = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi dx$$

or
$$\bar{p} = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx \quad (9)$$

and
$$\bar{E} = \int_{-\infty}^{\infty} \psi^* \hat{E} \psi dx = \int_{-\infty}^{\infty} \psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \psi dx$$

or
$$\bar{E} = i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial t} dx \quad (10)$$

Both equations can be evaluated for any acceptable wave function $\psi(x, t)$.

Q: (M/A 2005) Expectation values of the momentum operator is given by

$$\bar{p} = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi dx . \text{ Explain why it cannot be written as}$$

$$\int_{-\infty}^{\infty} \hat{p}\psi^*\psi dx \quad \text{and} \quad \int_{-\infty}^{\infty} \psi^*\psi \hat{p} dx$$

where \hat{p} is the operator.

Ans: The momentum operator \hat{p} is given by

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

Now considering the first case and using the operator we write

$$\int_{-\infty}^{\infty} \hat{p}\psi^*\psi dx = -i\hbar \int_{-\infty}^{\infty} \frac{\partial}{\partial x} \psi^*\psi dx = -i\hbar [\psi^*\psi]_{-\infty}^{\infty} = 0$$

Since ψ and ψ^* are zero at $x = \pm\infty$.

Now consider the second case then we write,

$$\int_{-\infty}^{\infty} \psi^*\psi \hat{p} dx = -i\hbar \int_{-\infty}^{\infty} \psi^*\psi \frac{\partial}{\partial x} dx$$

which has no sense.

Thus the equation for the expectation values of the momentum of the particle cannot be written as described by the last two cases.

5 Probability Current or Continuity equation:

Let us consider the motion of a particle between x_1 and x_2 in Fig. 1. Let S_1 be the flux of probability of existence of the particle or probability current at x_1 and S_2 be at x_2 . For probability density represented by $|\psi|^2$ to be conserved, any difference between S_1 and S_2 must be equal to the rate at which

the total probability $\int_{x_1}^{x_2} |\psi|^2 dx$ in the region between x_1 and x_2 is changing with time. i.e.,

$$\frac{\partial}{\partial t} \int_{x_1}^{x_2} |\psi|^2 dx = S_1 - S_2 \quad (1)$$

S_1 is positive as incoming and S_2 is negative as outgoing.

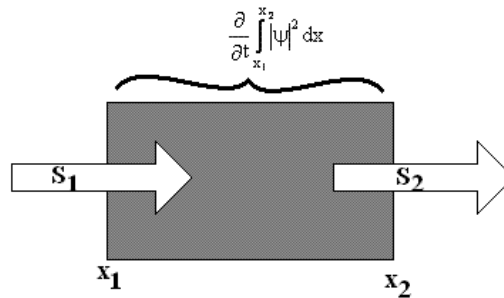


Fig. 1.

Proof: Consider the time-dependent Schrödinger's equation

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

and its complex conjugate which is obtained by replacing i by $-i$ and ψ by ψ^* such as

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + V\psi^* \quad (3)$$

Multiply (2) by ψ^* from left and (3) by ψ from right, we obtain

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

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

Subtracting second from first, we get

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

Which simplifies to

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

or
$$\frac{\partial}{\partial t}(\psi^*\psi) = \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$$

Integrating both sides of the equation from x_1 to x_2 , we get

$$\begin{aligned}\frac{\partial}{\partial t}\int_{x_1}^{x_2}(\psi^*\psi)dx &= \frac{i\hbar}{2m}\int_{x_1}^{x_2}\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)dx \\ \frac{\partial}{\partial t}\int_{x_1}^{x_2}(\psi^*\psi)dx &= \frac{i\hbar}{2m}\left[\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right]_{x_1}^{x_2} = -\frac{i\hbar}{2m}\left[\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right]_{x_2}^{x_1}\end{aligned}$$

(4)

Comparing it with equation (1), we get

$$S = -\frac{i\hbar}{2m}\left[\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right] \quad (5)$$

The minus sign is required in order that the right-hand side of equation (4) is $S_2 - S_1$.

Now consider the wave function ψ as

$$\psi = Ae^{-\frac{i}{\hbar}(Et - px)}$$

Which gives $\frac{\partial\psi}{\partial x} = \frac{i}{\hbar}p\psi$ and hence $\frac{\partial\psi^*}{\partial x} = -\frac{i}{\hbar}p\psi^*$. Substituting these in equation (5), we get

$$S = -\frac{i\hbar}{2m}\left[\frac{ip}{\hbar}\psi^*\psi + \frac{ip}{\hbar}\psi\psi^*\right]$$

or
$$S = \frac{p}{m}\psi^*\psi$$

since $\psi\psi^* = \psi^*\psi$

or
$$S = v|\psi|^2 \quad (6)$$

Since $p/m = v$, the speed of the particle. The probability current for a free particle is simply the product of its probability density and its speed. Equation (1) for the conservation of probability in this case can be written as

$$\frac{\partial}{\partial t}\int_{x_1}^{x_2}|\psi|^2 dx = |\psi|^2_1 v_1 - |\psi|^2_2 v_2 \quad (7)$$

This is same as the equation of conservation of mass in fluid mechanics except the probability density $|\psi|^2$ is in place of mass density ρ .

6 Schrödinger's equation: Steady state form or Time-independent form

In case of problems where potential energy of a particle depends on its position only, then the Schrödinger's wave equation may be simplified by removing all references to time. The Schrödinger's wave equation, whose solution is a position function only, is known as steady state form of Schrödinger's equation.

Consider the wave function $\psi(x, t)$ as

$$\psi(x, t) = Ae^{-\frac{i}{\hbar}(Et - px)} \quad (1)$$

Simplifying it we have

$$\psi(x, t) = Ae^{-\frac{i}{\hbar}Et} e^{\frac{i}{\hbar}px}$$

Considering the position dependent part as

$$\psi(x) = Ae^{\frac{i}{\hbar}px}$$

Then, equation (1) becomes

$$\psi(x, t) = e^{-\frac{i}{\hbar}Et} \psi(x) \quad (2)$$

Differentiating it with respect to x we get

$$\frac{\partial^2 \psi(x, t)}{\partial x^2} = e^{-\frac{i}{\hbar}Et} \frac{d^2 \psi(x)}{dx^2} \quad (3)$$

Similarly differentiating it with respect to time, we get

$$\frac{\partial \psi(x, t)}{\partial t} = \psi(x) \left(-\frac{i}{\hbar} E \right) e^{-\frac{i}{\hbar}Et} \quad (4)$$

The Schrödinger's time-dependent equation is

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V\psi(x, t) \quad (5)$$

Substituting equations (2), (3) and (4) in equation (5), we get

$$i\hbar \psi(x) \left(-\frac{i}{\hbar} E \right) e^{-\frac{i}{\hbar}Et} = -\frac{\hbar^2}{2m} e^{-\frac{i}{\hbar}Et} \frac{d^2 \psi(x)}{dx^2} + V\psi(x) e^{-\frac{i}{\hbar}Et}$$

or
$$E\psi(x) = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V\psi(x)$$

or
$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)]\psi(x) = 0 \quad (6)$$

The equation (6) is the Schrödinger's equation in steady state form in one dimension. In three dimensions, it becomes

$$\nabla^2 \psi(r) + \frac{2m}{\hbar^2} [E - V(r)]\psi(r) = 0 \quad (7)$$

7 Eigen values and Eigen functions:

In classical mechanics the total energy of a particle is given by the kinetic energy plus the potential energy. Thus

$$E = T + V$$

Similarly, in quantum mechanics the total energy operator, called Hamiltonian operator is denoted by \hat{H} , is given by the kinetic energy operator plus the potential energy operator. Thus,

$$\hat{H} = \hat{T} + \hat{V}$$

By substituting the values of the operators, we get

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (1)$$

Multiplying this equation by $\psi(x)$, we get

$$\hat{H}\psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) \quad (2)$$

Consider the Schrödinger's equation in steady state form

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

Rearranging it we get

$$E\psi(x) = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x)\psi(x) = 0 \quad (3)$$

Comparing equations (2) and (3), we have

$$\hat{H}\psi(x) = E\psi(x) \quad (4)$$

Equation (4) represents the Schrödinger's equation in steady state form in terms of the Hamiltonian operator. However, this equation can be solved for certain values of the energy E_n corresponding to certain wave function ψ_n . therefore, the Schrödinger's equation in steady state form can be written as

$$\hat{H}\psi_n = E\psi_n \quad (5)$$

These energy values E_n are called as eigen values or characteristic values or proper values. Corresponding to each eigen values there is a wave function ψ_n obtained as solution of equation (5). This function ψ_n is referred as eigen function or characteristic function or proper function.

8 Particle in One-Dimensional Box: Energy quantization and Wave function

Let us imagine that the motion of a freely moving particle of mass m along x -axis is restricted in the region (or box) formed by walls at $x = 0$ and $x = L$. It is assumed that there is no energy loss even after it collides with walls of box. Thus total energy of the particle is constant within the box. It is obvious that in present situation, potential energy is infinite on both sides of the box, while V is constant, say zero inside region of the box.

$$\begin{aligned} V(x) &= \infty & \text{for } x \geq 0 \text{ and } x \leq L & \quad (1a) \\ V(x) &= 0 & \text{for } 0 < x < L & \quad (1b) \end{aligned}$$

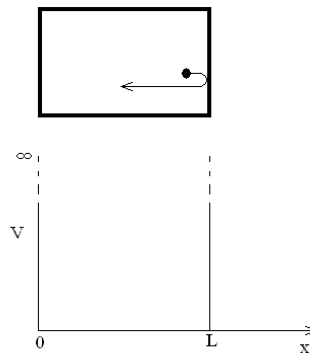


Fig. 1. A particle confined to a box of width L .

The motion of particle is limited to region inside the box, since the particle cannot have infinite amount of energy. Therefore the boundary condition for the wave function is

$$\psi(x) = 0 \quad \text{for } x \geq 0 \text{ and } x \leq L \quad (1c)$$

Consider the steady state form of Schrödinger's equation we have

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

Applying boundary condition (1b), we have

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad (3)$$

$$\text{Let } k^2 = \frac{2mE}{\hbar^2} \quad (4)$$

then we get

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad (5)$$

This is standard differential equation, which has two possible solutions

$$\psi = A\sin(kx) \quad (6a)$$

$$\psi = B\cos(kx) \quad (6b)$$

Equation (6b) is not an acceptable solution, because it does not satisfy boundary condition that $\psi = 0$ at $x = 0$ and $x = L$, Since $\cos(0) = 1$. To make it acceptable, it is required that $B=0$. However, equation (6a) is the acceptable solution of equation (5) because it satisfy the boundary conditions that $\psi = 0$ at $x = 0$ and $\psi = 0$ at $x = L$, provided

$$kL = n\pi \quad (7)$$

where $n = 1, 2, 3, \dots$

Substituting the value of k from equation (4) in equation (7), we get

$$\frac{\sqrt{2mE}}{\hbar} L = n\pi \quad (8)$$

Writing E as E_n and simplifying equation (8), we have

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad (9)$$

This equation (9) implies that the energy of the particle can have only certain values, which are known as eigen values. These are specifically represented as E_n instead of E . The integer n corresponding to energy eigen value E_n is called as its quantum number. It may be also noted that the particle in box cannot have zero energy. This result is arisen due to fact that the wave function is finite and exist some where in box at all times. If the particle has zero energy then the wave function ψ would be zero everywhere in the box.

Substituting the value of k from equation (7) in equation (6a), we get the wave function as

$$\psi_n = A \sin\left(\frac{n\pi}{L} x\right) \quad (11)$$

Clearly for each quantum number n , ψ_n is a single-valued function and ψ_n and $\partial\psi_n/\partial x$ are continuous. Further it should meet to the requirement of normalization. That is, if ψ_n is to be normalized wave function then

$$\begin{aligned} \int_{-\infty}^{\infty} |\psi_n|^2 dx &= \int_0^L |\psi_n|^2 dx = 1 \\ A^2 \int_0^L \sin^2\left(\frac{n\pi}{L} x\right) dx &= 1 \\ A^2 \frac{L}{2} &= 1 \\ A &= \sqrt{\frac{2}{L}} \end{aligned} \quad (12)$$

Thus the normalized wave functions are

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \quad (13)$$

where $n = 1, 2, 3, \dots$

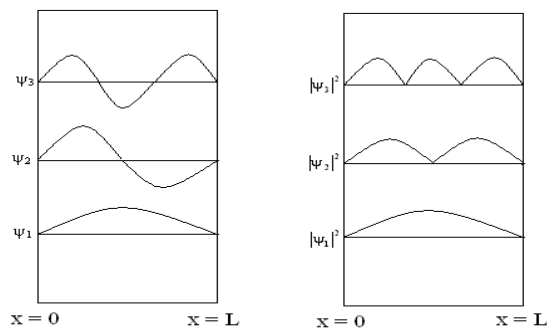


Fig. 2. Wave functions and probability densities of a particle in a box.

The normalized wave functions ψ_1 , ψ_2 , and ψ_3 together with probability densities $|\psi_1|^2$, $|\psi_2|^2$ and $|\psi_3|^2$ are plotted in figure 2. While ψ_n may be positive as well as negative, $|\psi_n|^2$ is always positive and is equal to the probability p of finding the particle there. In every case $|\psi_n|^2 = 0$ at $x = 0$ and $x = L$, the boundaries of the box. At a particular point in the box the probability of the particle being present may be very different for different quantum numbers. For instance, particle at lowest energy level of $n = 1$ is

most likely to be in the middle of the box, while a particle in the next higher state of $n = 2$ is never there. Classical physics, of course, predicts the same probability for the particle being anywhere in the box.

9 Particle in One-Dimensional Box: Momentum quantization and Momentum wave function

The wave function of a particle trapped in one-dimensional box of length L is given by

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \quad (1)$$

where, $n = 1, 2, 3, \dots$

The energy associated with the particle is given by

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad (2)$$

Here ψ_n is called energy eigen function corresponding to energy eigen value E_n . As the potential energy of the particle inside the box is zero, equation (2) gives the kinetic energy of the particle.

Further the momentum and energy are related by

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

or
$$E_n = \frac{p_n^2}{2m}$$

or
$$p_n \pm \sqrt{2mE_n}$$

Using equation (2), we get

$$p_n = \pm \frac{n\pi\hbar}{L} \quad (3)$$

Thus
$$p_n^+ = + \frac{n\pi\hbar}{L} \quad (4a)$$

$$p_n^- = - \frac{n\pi\hbar}{L} \quad (4b)$$

Thus there can be two momentum eigen values corresponding to every energy eigen function. When the particle moves along +ve direction of x-axis, it has p_n^+ momentum and when it moves along -ve direction possesses p_n^- momentum. The average value of the momentum is zero.

Let us check whether the wave function given by equation (1) can work as the momentum eigen function. The momentum eigen equation is written as

$$\hat{p}\psi_n = P_n\psi_n \quad (5)$$

Further the momentum operator is given by

$$\hat{p} = -i\hbar \frac{d}{dx} \quad (6)$$

To check we calculate

$$\hat{p}\psi_n = -i\hbar \frac{d}{dx} \left(\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \right) = -\frac{i\hbar n\pi}{L} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi}{L} x\right) \neq P_n\psi_n \quad (7)$$

Thus equation (1) is not a momentum eigen function. To obtain correct momentum eigen function, we use the following identity in equation (1)

$$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$$

$$\psi_n = \frac{1}{2i} \sqrt{\frac{2}{L}} \left(e^{\frac{in\pi}{L} x} - e^{-\frac{in\pi}{L} x} \right)$$

This gives

$$\psi_n^+ = \frac{1}{2i} \sqrt{\frac{2}{L}} \left(e^{\frac{in\pi}{L}x} \right) \quad (8a)$$

$$\text{and } \psi_n^- = \frac{1}{2i} \sqrt{\frac{2}{L}} \left(e^{-\frac{in\pi}{L}x} \right) \quad (8b)$$

Now we calculate

$$\begin{aligned} \hat{p}\psi_n^+ &= -i\hbar \frac{d}{dx} \left[\frac{1}{2i} \sqrt{\frac{2}{L}} \left(e^{\frac{in\pi}{L}x} \right) \right] = -i\hbar \frac{in\pi}{L} \left[\frac{1}{2i} \sqrt{\frac{2}{L}} \left(e^{\frac{in\pi}{L}x} \right) \right] \\ &= \frac{n\pi\hbar}{L} \left[\frac{1}{2i} \sqrt{\frac{2}{L}} \left(e^{\frac{in\pi}{L}x} \right) \right] \end{aligned}$$

$$\text{or } \hat{p}\psi_n^+ = \frac{n\pi\hbar}{L} \psi_n^+ = p_n^+ \psi_n^+ \quad (9a)$$

Similarly, we get

$$\hat{p}\psi_n^- = -\frac{n\pi\hbar}{L} \psi_n^- = p_n^- \psi_n^- \quad (9b)$$

Thus p_n^+ and p_n^- given by equations (4) are the momentum eigen values corresponding to momentum eigen functions ψ_n^+ and ψ_n^- given by equations (8) respectively. Clearly, the momentum eigen values are quantized like energy eigen values.